STN Structure Search (Reg / Caplus)

10/526,851 07/07/2007,

Connecting via Winsock to STN

Search Strategy

Claim 1

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | MAR 15 | WPIDS/WPIX enhanced with new FRAGHITSTR display format |
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| NEWS 4 | MAR 20 | MARPAT now updated daily |
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| NEWS 14 | MAY 14 | RDISCLOSURE on STN Easy enhanced with new search and display fields |
| NEWS 15 | MAY 21 | BIOSIS reloaded and enhanced with archival data |
| NEWS 16 | MAY 21 | TOXCENTER enhanced with BIOSIS reload |
| NEWS 17 | MAY 21 | CA/CAplus enhanced with additional kind codes for German patents |
| NEWS 18 | MAY 22 | CA/CAplus enhanced with IPC reclassification in Japanese patents |
| NEWS 19 | JUN 27 | CA/CAplus enhanced with pre-1967 CAS Registry Numbers |
| NEWS 20 | JUN 29 | STN Viewer now available |
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NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

| | |
|---|---|
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS IPC8 | For general information regarding STN implementation of IPC 8 |

Enter NEWS followed by the item number or name to see news on that specific topic.

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of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:55:30 ON 07 JUL 2007

=> fil reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:55:43 ON 07 JUL 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 JUL 2007 HIGHEST RN 941372-96-9
DICTIONARY FILE UPDATES: 5 JUL 2007 HIGHEST RN 941372-96-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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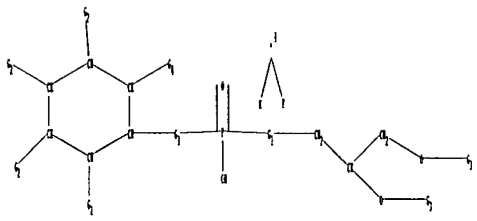
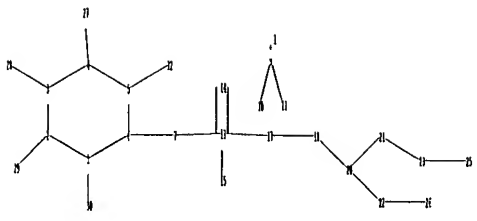
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 1.str





chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

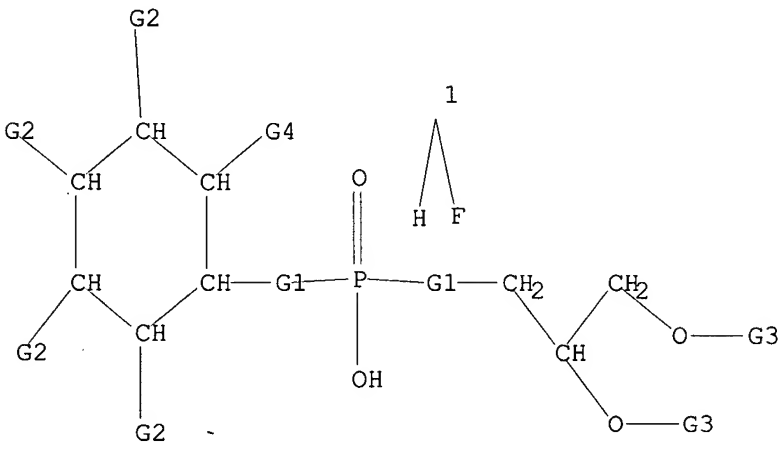
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:56:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 279 TO ITERATE

100.0% PROCESSED 279 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4578 TO 6582
PROJECTED ANSWERS: 672 TO 1568

L2 50 SEA SSS SAM L1

=> d scan

```
=> d his

     (FILE 'HOME' ENTERED AT 10:55:30 ON 07 JUL 2007)

     FILE 'REGISTRY' ENTERED AT 10:55:43 ON 07 JUL 2007
L1              STRUCTURE UPLOADED
L2           50 S L1

=> s l1 full
FULL SEARCH INITIATED 10:56:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     5758 TO ITERATE

100.0% PROCESSED     5758 ITERATIONS                          1332 ANSWERS
SEARCH TIME: 00.00.01

L3         1332 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               172.55     172.76

FILE 'CAPLUS' ENTERED AT 10:56:50 ON 07 JUL 2007
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FILE COVERS 1907 - 7 Jul 2007  VOL 147 ISS 3
FILE LAST UPDATED: 6 Jul 2007  (20070706/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4         561 L3

=> d ibib abs hitstr 500-561
```

STN (Reg/Caplus)
Structure Search.



dependent Claims 18-27

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:21:25 ON 07 JUL 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 12:21:47 ON 07 JUL 2007
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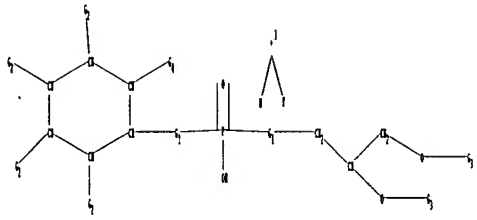
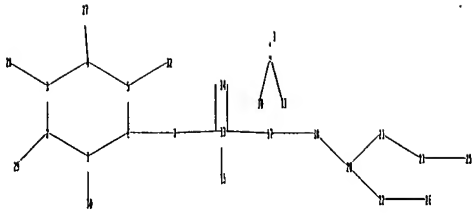
=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 1.str





chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
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1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
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1-30 2-29 3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
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1-2 1-6 2-3 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

G3:Cb,Ak

G4:H,O

Match level :
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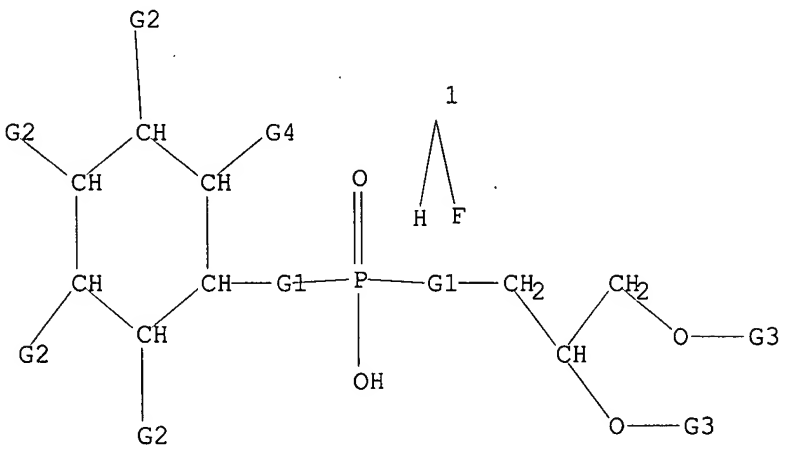
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

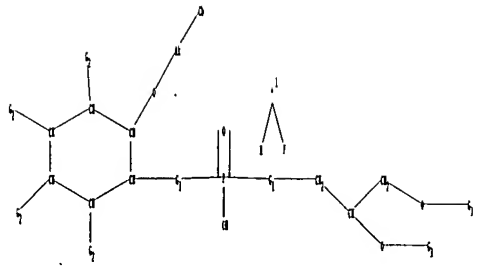
Structure attributes must be viewed using STN Express query preparation.

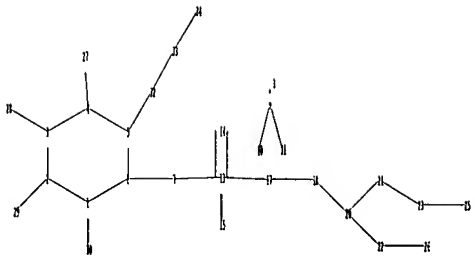
=> s l1 full
FULL SEARCH INITIATED 12:22:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5758 TO ITERATE

100.0% PROCESSED 5758 ITERATIONS 1332 ANSWERS
SEARCH TIME: 00.00.01

L2 1332 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claims 18 19.str





chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32 33
34
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25 32-33 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
32-33 33-34
exact bonds :
1-2 1-6 2-3 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

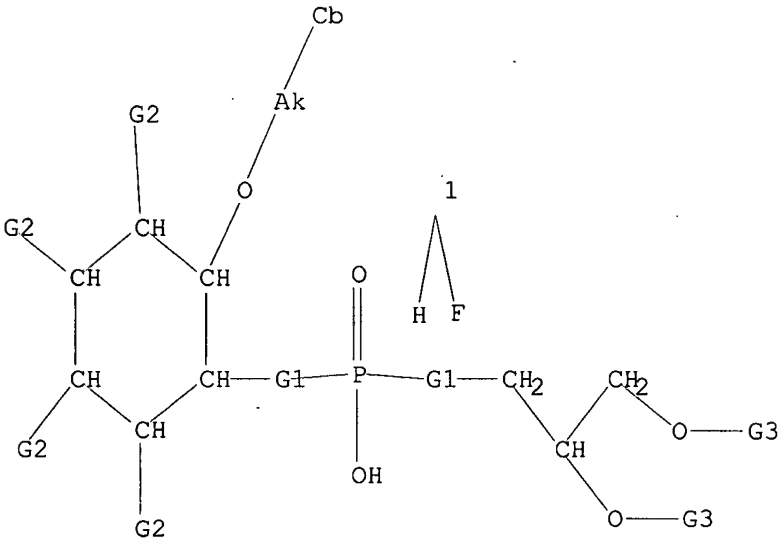
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS 33:CLASS 34:Atom

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l3 full sub=L2
FULL SUBSET SEARCH INITIATED 12:22:37 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1302 TO ITERATE

100.0% PROCESSED 1302 ITERATIONS 113 ANSWERS
SEARCH TIME: 00.00.01

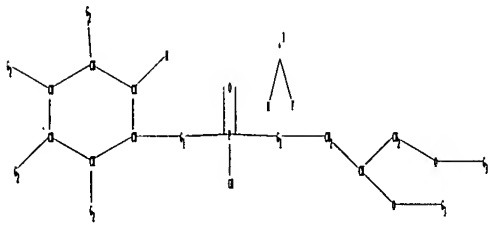
L4 113 SEA SUB=L2 SSS FUL L3

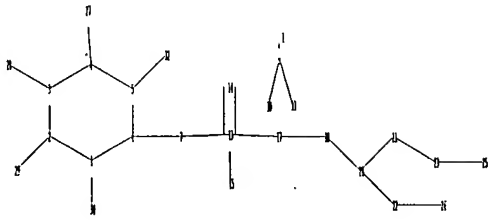
```
=> d his

     (FILE 'HOME' ENTERED AT 12:21:25 ON 07 JUL 2007)

     FILE 'REGISTRY' ENTERED AT 12:21:47 ON 07 JUL 2007
L1             STRUCTURE UPLOADED
L2          1332 S L1 FULL
L3             STRUCTURE UPLOADED
L4           113 S L3 FULL  SUB=L2

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 20.str
```





```
chain nodes :
7  9  10  11  13  14  15  17  18  20  21  22  23  25  26  27  28  29  30  32
ring nodes :
1  2  3  4  5  6
chain bonds :
1-30  2-29  3-28  4-27  5-32  6-7  7-13  9-10  9-11  13-14  13-15  13-17  17-18
18-20  20-21  20-22  21-23  22-26  23-25
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-30  2-29  3-28  4-27  5-6  6-7  7-13  13-17  17-18  20-22  22-26  23-25
exact bonds :
1-2  1-6  2-3  3-4  4-5  5-32  9-10  9-11  18-20  20-21  21-23
```

normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

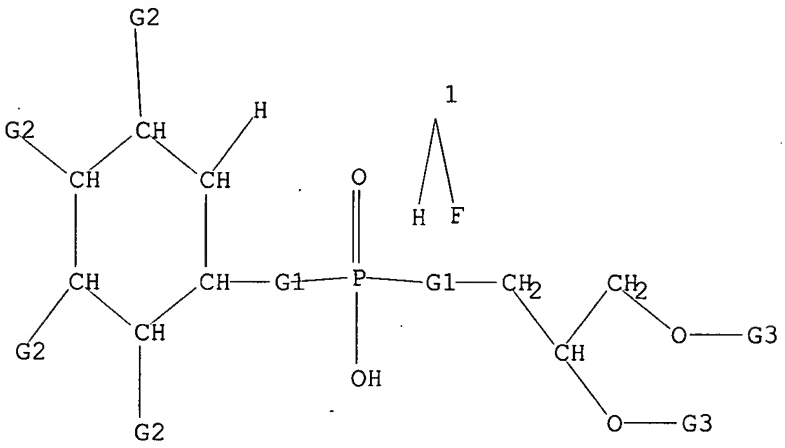
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

Structure attributes must be viewed using STN Express query preparation.

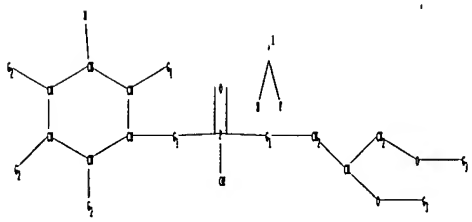
=> s l5 full sub=l2
FULL SUBSET SEARCH INITIATED 12:25:56 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

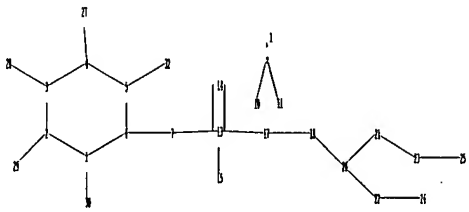
```
=> d his

     (FILE 'HOME' ENTERED AT 12:21:25 ON 07 JUL 2007)

     FILE 'REGISTRY' ENTERED AT 12:21:47 ON 07 JUL 2007
L1             STRUCTURE UPLOADED
L2          1332 S L1 FULL
L3             STRUCTURE UPLOADED
L4           113 S L3 FULL  SUB=L2
L5             STRUCTURE UPLOADED
L6            30 S L5 FULL  SUB=L2

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 21.str
```





```
chain nodes :
7  9  10  11  13  14  15  17  18  20  21  22  23  25  26  27  28  29  30  32
ring nodes :
1  2  3  4  5  6
chain bonds :
1-30  2-29  3-28  4-27  5-32  6-7  7-13  9-10  9-11  13-14  13-15  13-17  17-18
18-20  20-21  20-22  21-23  22-26  23-25
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-30  2-29  3-28  5-6  5-32  6-7  7-13  13-17  17-18  20-22  22-26  23-25
exact bonds :
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normalized bonds :
13-14  13-15
```

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G2:H,OH

G3:Cb,Ak

G4:H,O

Match level :
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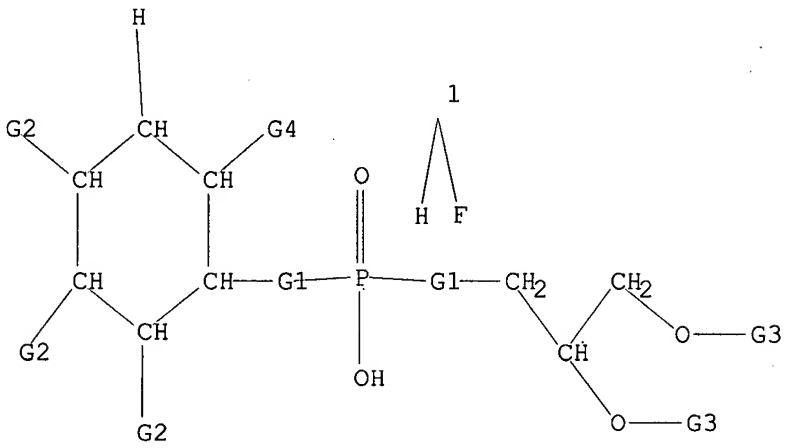
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

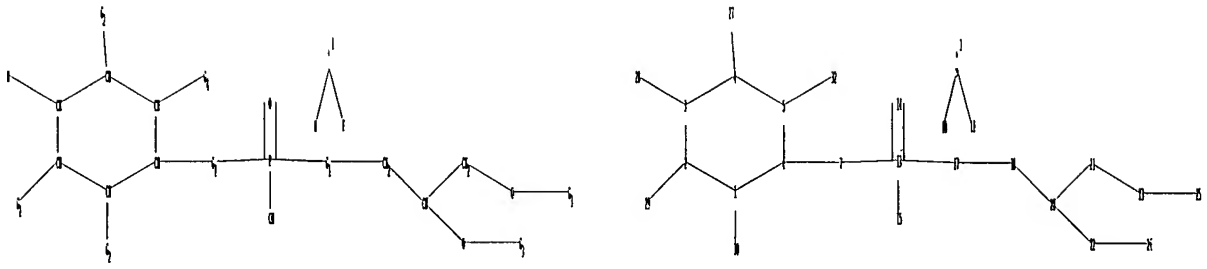
Structure attributes must be viewed using STN Express query preparation.

=> s l7 full sub=L2
FULL SUBSET SEARCH INITIATED 12:27:36 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 60 ANSWERS
SEARCH TIME: 00.00.01

L8 60 SEA SUB=L2 SSS FUL L7

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 22.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 3-4 3-28 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

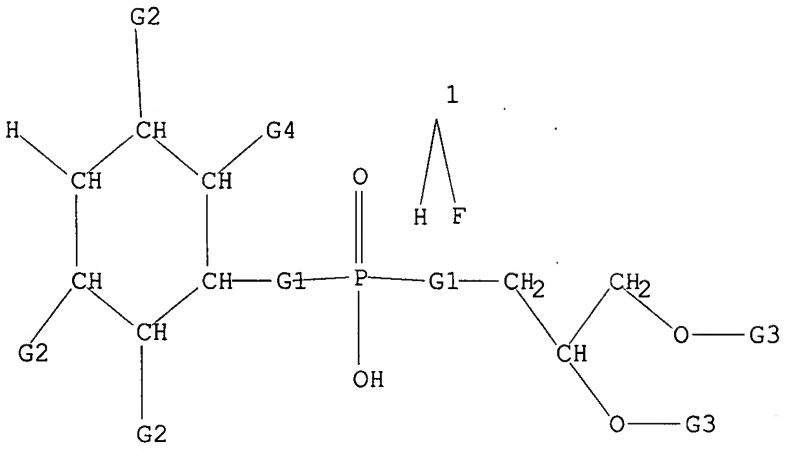
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L9 STRUCTURE UPLOADED

=> d
L9 HAS NO ANSWERS
L9 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

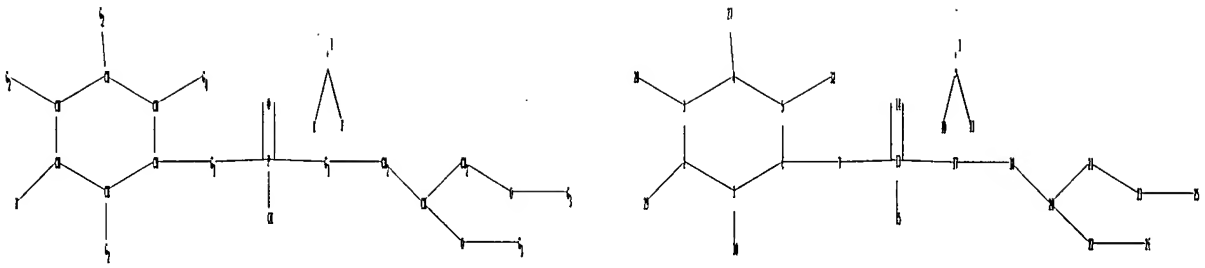
Structure attributes must be viewed using STN Express query preparation.

=> s l9 full sub=L2
FULL SUBSET SEARCH INITIATED 12:28:08 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L10 8 SEA SUB=L2 SSS FUL L9

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 23.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 2-29 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

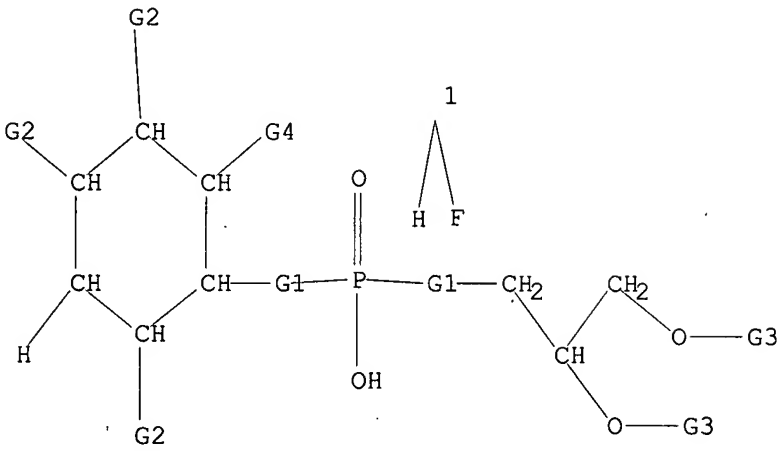
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L11 STRUCTURE UPLOADED

=> d
L11 HAS NO ANSWERS
L11 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

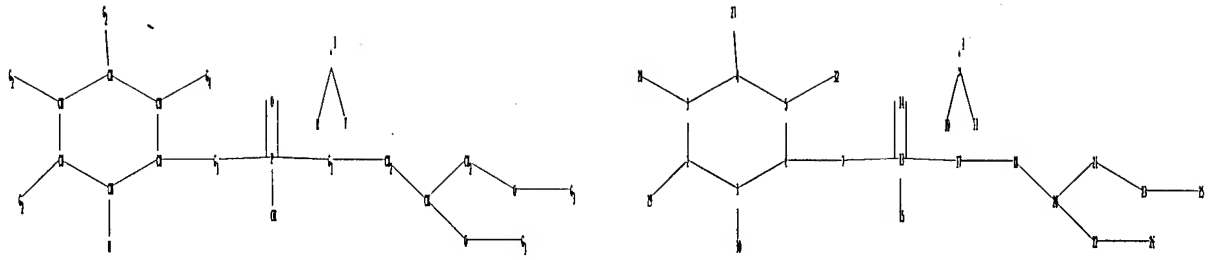
Structure attributes must be viewed using STN Express query preparation.

=> s l11 full sub=L2
FULL SUBSET SEARCH INITIATED 12:28:35 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 60 ANSWERS
SEARCH TIME: 00.00.01

L12 60 SEA SUB=L2 SSS FUL L11

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 24.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-29 3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 1-30 2-3 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

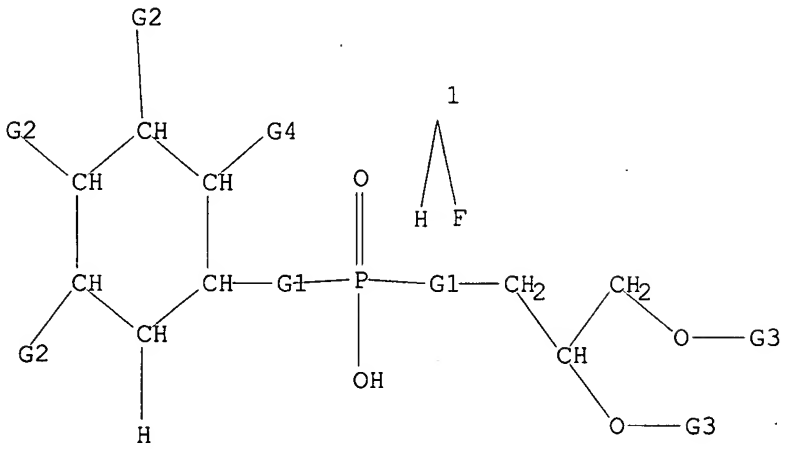
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L13 STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

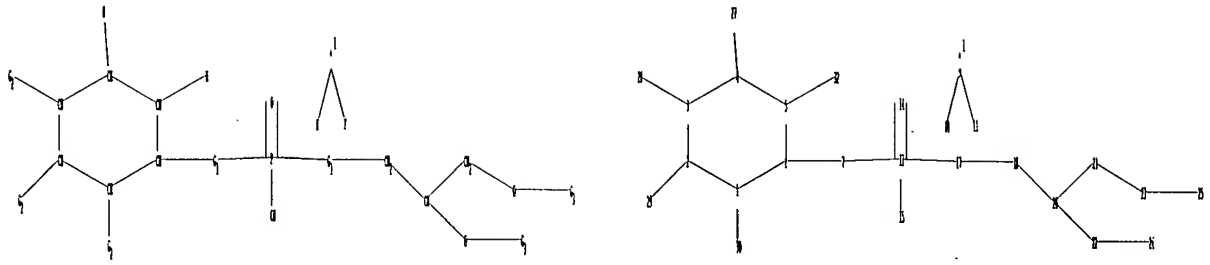
Structure attributes must be viewed using STN Express query preparation.

=> s l13 full sub=L2
FULL SUBSET SEARCH INITIATED 12:29:12 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 30 ANSWERS
SEARCH TIME: 00.00.01

L14 30 SEA SUB=L2 SSS FUL L13

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 25.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 3-28 5-6 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 3-4 4-5 4-27 5-32 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

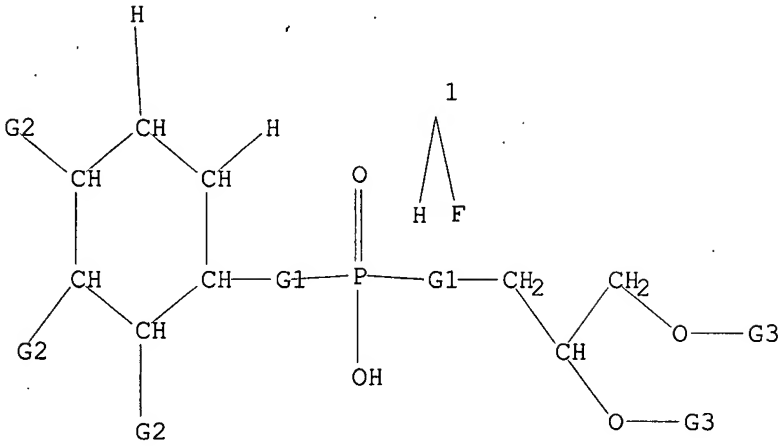
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L15 STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

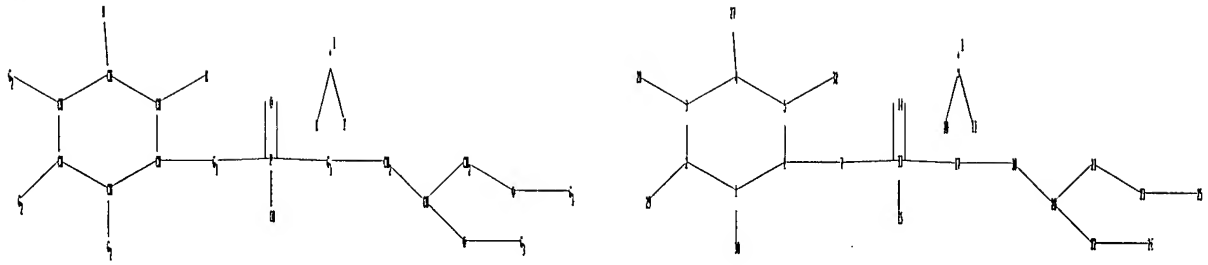
Structure attributes must be viewed using STN Express query preparation.

=> s l15 full sub=L2
FULL SUBSET SEARCH INITIATED 12:29:52 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L16 24 SEA SUB=L2 SSS FUL L15

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 25.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 3-28 5-6 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 3-4 4-5 4-27 5-32 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

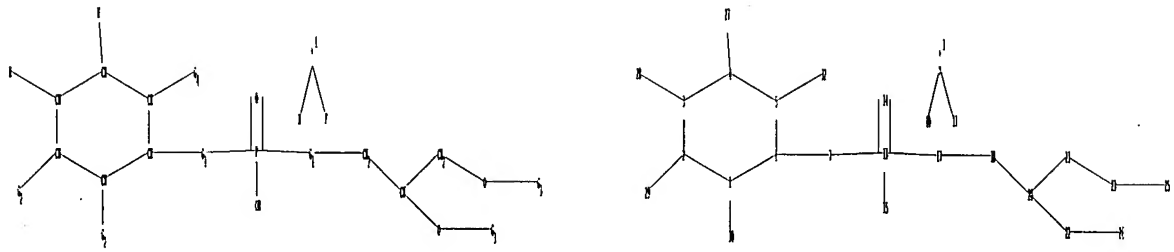
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L17 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 26.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-30 2-29 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 2-3 3-4 3-28 4-5 4-27 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

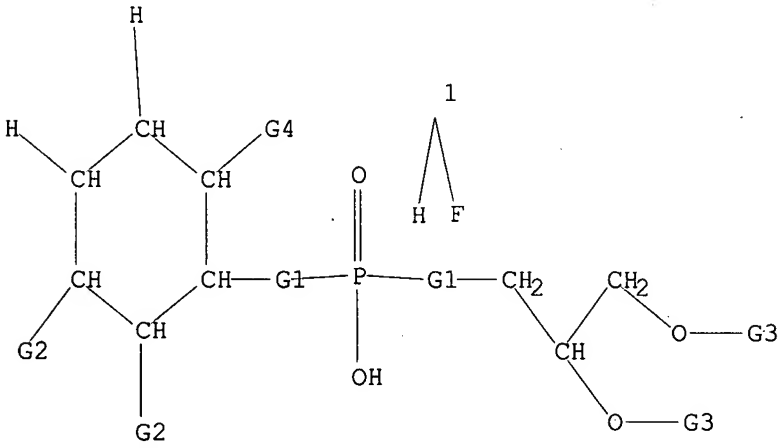
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L18 STRUCTURE UPLOADED

=> d
L18 HAS NO ANSWERS
L18 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

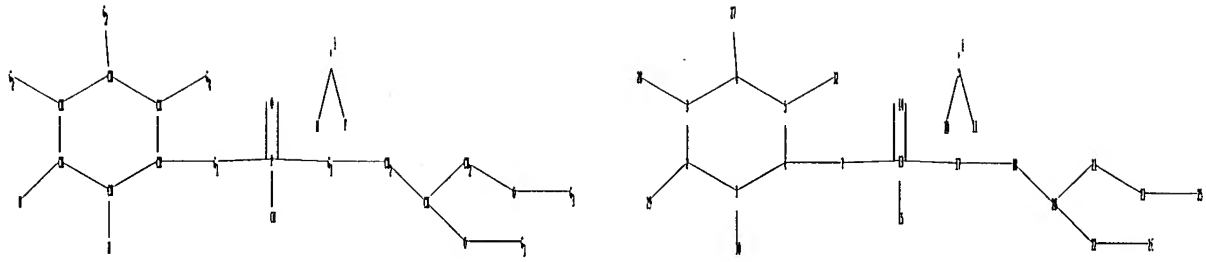
Structure attributes must be viewed using STN Express query preparation.

=> s l18 full sub=L2
FULL SUBSET SEARCH INITIATED 12:30:42 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L19 7 SEA SUB=L2 SSS FUL L18

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\July claim 27.str



chain nodes :
7 9 10 11 13 14 15 17 18 20 21 22 23 25 26 27 28 29 30 32
ring nodes :
1 2 3 4 5 6
chain bonds :
1-30 2-29 3-28 4-27 5-32 6-7 7-13 9-10 9-11 13-14 13-15 13-17 17-18
18-20 20-21 20-22 21-23 22-26 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
3-28 4-27 5-6 5-32 6-7 7-13 13-17 17-18 20-22 22-26 23-25
exact bonds :
1-2 1-6 1-30 2-3 2-29 3-4 4-5 9-10 9-11 18-20 20-21 21-23
normalized bonds :
13-14 13-15

G1:O,CH2,CF2,[*1]

G2:H,OH

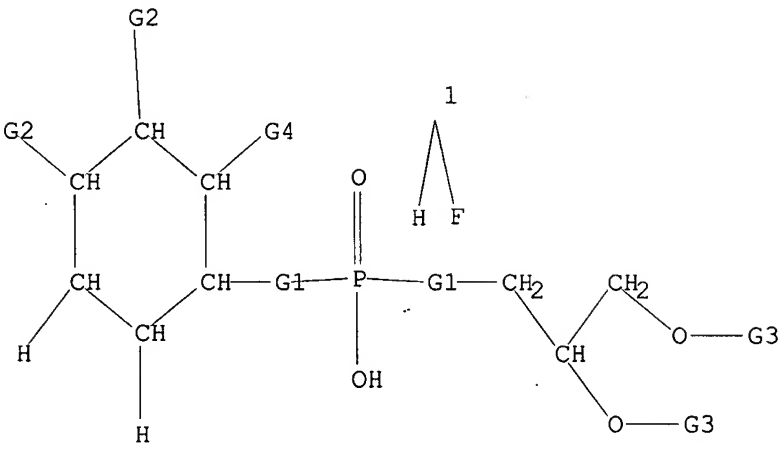
G3:Cb,Ak

G4:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
32:CLASS

L20 STRUCTURE UPLOADED

=> d
L20 HAS NO ANSWERS
L20 STR




G1 O,CH2,CF2,[@1]

G2 H,OH

G3 Cb,Ak

G4 H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l20 full sub=L2
FULL SUBSET SEARCH INITIATED 12:31:11 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1332 TO ITERATE

100.0% PROCESSED 1332 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L21 24 SEA SUB=L2 SSS FUL L20

=> d his

(FILE 'HOME' ENTERED AT 12:21:25 ON 07 JUL 2007)

FILE 'REGISTRY' ENTERED AT 12:21:47 ON 07 JUL 2007
L1 STRUCTURE UPLOADED
L2 1332 S L1 FULL
L3 STRUCTURE UPLOADED
L4 113 S L3 FULL SUB=L2
L5 STRUCTURE UPLOADED
L6 30 S L5 FULL SUB=L2

```
L7              STRUCTURE UPLOADED
L8           60 S L7 FULL  SUB=L2
L9              STRUCTURE UPLOADED
L10           8 S L9 FULL  SUB=L2
L11             STRUCTURE UPLOADED
L12          60 S L11 FULL  SUB=L2
L13             STRUCTURE UPLOADED
L14          30 S L13 FULL  SUB=L2
L15             STRUCTURE UPLOADED
L16          24 S L15 FULL  SUB=L2
L17             STRUCTURE UPLOADED
L18             STRUCTURE UPLOADED
L19           7 S L18 FULL  SUB=L2
L20             STRUCTURE UPLOADED
L21          24 S L20 FULL  SUB=L2

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             544.70     544.91

FILE 'CAPLUS' ENTERED AT 12:31:29 ON 07 JUL 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 7 Jul 2007  VOL 147 ISS 3
FILE LAST UPDATED: 6 Jul 2007  (20070706/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l4                    Claims 18+19
L22          47 L4

=> s l6
L23          27 L6                 20

=> s l8
L24          32 L8                 21

=> s l10
L25           7 L10                22
```

claims 23

```
=> s l12
L26          32 L12

=> s l14
L27          27 L14

=> s l16
L28          22 L16

=> s l19
L29           7 L19

=> s l21
L30          22 L21

=> s l22-l30
L31          77 (L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR L28 OR L29 OR L30)

=> d ibib abs hitstr 1-77
```

L31 ANSWER 1 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:201063 CAPLUS
DOCUMENT NUMBER: 146:270775
TITLE: Neuregulin1 (NRG1)-stimulated chemotaxis of B lymphocytes and uses in diagnosis and drug screening for schizophrenia and cancer
INVENTOR(S): Weinberger, Daniel R.; Kanakry, Christopher G.; Ren-Patterson, Renee; Sei, Yoshitatsu
PATENT ASSIGNEE(S): The Government of the United States of America, As Represented by the Secretary, Department of Health and Human Services, USA
SOURCE: PCT Int. Appl., 102pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2007021853 | A2 | 20070222 | WO 2006-US31217 | 20060811 |

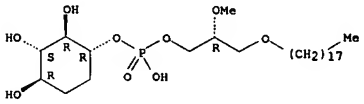
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

| | | |
|---|---|---|
| PRIORITY APPLN. INFO.: | US 2005-707714P | P 20050812 |
| | US 2005-735353P | P 20051110 |

AB The invention includes methods for detecting or measuring lymphocyte chemotaxis comprising detecting or measuring the migration of lymphocytes in a direction toward an increased level of a chemoattractant, wherein said chemoattractant is neuregulin1 (NRG1) or epidermal growth factor (EGF)-like domain thereof or derivs. or analogs thereof, wherein the presence and amount of said migration of lymphocytes indicates the presence and amount, resp., of lymphocyte chemotaxis. The invention also includes methods of diagnosing schizophrenia and other brain disorders that involve genetic defects in NRG1 signaling pathways and cancers that involve overexpression of ErbB/Her receptors, methods for identifying lymphocyte chemoattractants and tumor-derived cell chemotaxis antagonists and methods of making lymphocyte chemoattractants and tumor-derived cell chemotaxis antagonists. The inventors showed that B lymphoblasts expressed erbB2 and erbB3 receptors and that NRG1α signaled through these receptors via the PI3K/Akt and PLC pathways in order to promote chemotactic migration. Thus NRG-ErbB signaling in B lymphoblasts was analogous to that in neuronal cells. NRG1-ErbB signaling was examd. in patients with schizophrenia using EBV-transformed B lymphoblasts. Genetic variation in NRG1 that was previously assocd. with schizophrenia predicted the migratory response of the B lymphoblasts to NRG1. NRG1α induced an oscillatory pattern of cell attachment and detachment as measured in an adhesion assay. The amplitude of the oscillation correlated with the effectiveness of NRG1α-induced cell migration. The NRG1α-induced oscillation of cell adhesion was dependent on erbB2/PI3K/Akt signaling, with Akt1 showing a direct phys. interaction with the CD11a/CD18 integrin expressed in lymphoblasts. The amplitude of oscillation was lower in B lymphoblast derived from schizophrenics compared with those derived from normal controls. The amplitude of oscillation was also related to two genes implicated in schizophrenia, catechol-O-methyltransferase (COMT) and NRG1.

IT 701976-55-8, Akt inhibitor III
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(neuregulin1 (NRG1)-stimulated chemotaxis of B lymphocytes and uses in diagnosis and drug screening for schizophrenia and cancer)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.

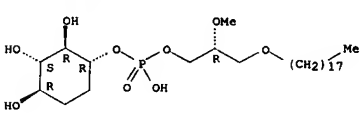


L31 ANSWER 2 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:164406 CAPLUS
DOCUMENT NUMBER: 146:311243
TITLE: Development of a microscopy-based assay for protein kinase Cζ activation in human breast cancer cells
AUTHOR(S): Zhao, Caijie; Cai, Mi; Zhang, Yao; Liu, Ying; Sun, Ronghua; Zhang, Ning
CORPORATE SOURCE: Beijing National Laboratory for Molecular Sciences, Department of Chemical Biology and State Key Laboratory of Molecular Dynamic and Stable Structures, College of Chemistry, Peking University, Beijing, 100871, Peop. Rep. China
SOURCE: Analytical Biochemistry (2007), 362(1), 8-15
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Protein kinase Cζ (PKCζ) plays a critical role in cancer cell chemotaxis. Upon activation induced by epidermal growth factor (EGF) or chemoattractant SDF-1α, PKCζ redistributes from cytosol to plasma membrane. Based on this property, we developed a rapid cell-based assay for inhibitors of ligand-induced PKCζ activation. PKCζ green fluorescent protein (GFP) was transfected into human breast cancer cells, MDA-MB-231, to establish a stable cell line, PKCζ-GFP/MDA-MB-231. PKCζ-GFP/MDA-MB-231 maintained phenotypes, such as chemotaxis, adhesion, and cell migration, similar to those of its parental cell line. Therefore it could be used as a representative cancer cell line. EGF induced translocation of PKCζ-GFP to plasma membrane in a pattern similar to that of endogenous PKCζ, indicative of activation of PKCζ Translocation of PKCζ-GFP could be easily and directly recorded by an inverted fluorescence microscope. Inhibitors of chemotaxis also impaired the translocation of PKCζ-GFP, which further validated the biol. relevance of our assay. Taken together, we have developed a simple, rapid, and reliable assay to detect the ligand-induced activation of PKCζ in human cancer cells. This assay can be used in screening for inhibitors of PKCζ activation, which is critically required for cancer cell chemotaxis.

IT 701976-55-8, Akt inhibitor III
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(assay in breast cancer cells to screen inhibitors of EGF/SDF-1α-induced protein kinase Cζ activation)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS

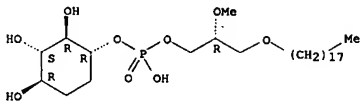
L31 ANSWER 1 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L31 ANSWER 2 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1324644 CAPLUS
DOCUMENT NUMBER: 146:197954
TITLE: Cotreatment with a novel phosphoinositide analogue inhibitor and carmustine enhances chemotherapeutic efficacy by attenuating AKT activity in gliomas
AUTHOR(S): Van Meter, Timothy E.; Broaddus, William C.; Cash, Dana; Fillmore, Helen
CORPORATE SOURCE: Department of Neurosurgery, Medical College of Virginia Campus, Virginia Commonwealth University, Richmond, VA, USA
SOURCE: Cancer (Hoboken, NJ, United States) (2006), 107(10), 2446-2454
CODEN: CANCAR; ISSN: 0008-543X
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Backround: Heightened activity of the AKT signaling pathway is prominent in malignant gliomas and has been suggested to play a role in treatment resistance. Selective targeting of AKT, therefore, may increase chemosensitivity. Recently, a novel class of AKT-selective inhibitors has been described, including SH-6, a phosphatidylinositol analog. Methods: The effects of SH-6 on AKT signaling were tested in glioma cells, and the putative role of AKT signaling in chemoresistance was tested by attenuating AKT signaling pharmacol. and genetically. The initial characterization of SH-6 included treatment of glioma cells with increasing doses of SH-6 (0.30-30 μM) and examining the effects on AKT signaling proteins by Western blot analyses and in kinase assays with immunopptd. AKT1. Dose-response studies with SH-6 administered to glioma cell lines were performed using a luminescent cell-viability assay (0.1-30 μM). Studies examining the effect of carmustine, either alone or in combination with either the phosphatidylinositol 3-kinase inhibitor LY294002 or SH-6, were performed by cell viability assays and clonogenic survival assays. The effect of carmustine on AKT activity as a response to treatment also was examined Caspase assays were used to examine the potential role of apoptosis in SH-6/carmustine-elicited cell death. Finally, the induction of a dominant-neg. AKT1 transgene was used in combination with carmustine to demonstrate the role of AKT1 in carmustine chemoresistance. Results: Serum-stimulated phosphorylation of AKT1 was inhibited by SH-6 at doses ≥10 μM (>70% decrease in Threonine 308 and Serine 473 phosphorylation of AKT1). In ATP assays, 72 h of treatment with SH-6 led to 50% LDs near 10 μM for 2 cell lines tested. SH-6 enhancement of carmustine-mediated cell death led to synergistic increases in Caspase 3/Caspase 7 activity, implicating apoptosis as the cell death mechanism. In clonogenic assays, SH-6 cotreatment with carmustine significantly decreased the number of colonies at 10 μM ($P < .05$) compared with carmustine alone. No decrease was observed in cells that were treated with SH-6 alone (10 μM). LY294002 (10 μM) was also able to enhance the effects of carmustine significantly in both cell lines. Conclusions: In the current study, the authors characterized the efficacy of a new class of adjuvant chemotherapeutics that show promise in enhancing the efficacy of standard chemotherapy regimens in gliomas.

L31 ANSWER 3 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 701976-55-8, SH 6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SH 6; cotreatment with phosphatidylinositol analog inhibitor, SH-6 and carmustine enhances chemotherapeutic efficacy by attenuating AKT activity in glioma cells)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

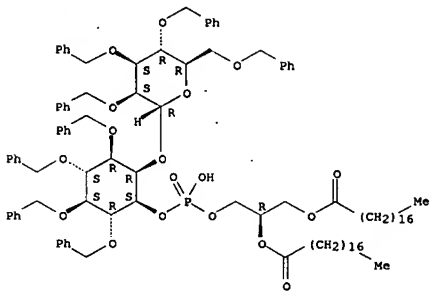
L31 ANSWER 4 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:678907 CAPLUS
DOCUMENT NUMBER: 145:306192
TITLE: Phosphatidylinositol mannosides: Synthesis and suppression of allergic airway disease
AUTHOR(S): Ainge, Gary D.; Hudson, Jennifer; Larsen, David S.; Painter, Gavin F.; Gill, Gurmit Singh; Harper, Jacquie L.
CORPORATE SOURCE: Industrial Research Limited, Lower Hutt, 31-310, N. Z.
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(16), 5632-5642
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:306192
AB Phosphatidylinositol mannoside (PIM) exts. from mycobacteria have been shown previously to suppress allergic airway inflammation in mice. To help determine the structural requirements for activity, PIM12 (1), PIM16 (2) and PIM2 (3) were synthesized and tested for their ability to suppress cellular inflammation in a mouse model of allergic asthma. The synthetic PIMs were all effective in suppressing airway eosinophilia in the asthma model, with PIM16 being the most effective. Suppression of all inflammatory cells monitored was observed, indicating a general blockade of cellular inflammation. Non-mannosylated phosphatidylinositol (PI) had no suppressive effect, indicating that at least one α-D-mannopyranosyl residue is necessary for activity. The suppressive effect of the three PIM compds. indicates that other members of this set may be of value in treatment of a range of diseases driven by infiltration of inflammatory cells.
IT 908853-72-5P 908853-77-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phosphatidylinositol mannosides preparation and suppression of allergic airway disease)
RN 908853-72-5 CAPLUS
CN D-myo-Inositol, 3,4,5,6-tetrakis-O-(phenylmethyl)-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, hydrogen (2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl phosphate, compd. with N,N-diethylethanamine (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 908853-71-4
CMF C107 H145 O18 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 4 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

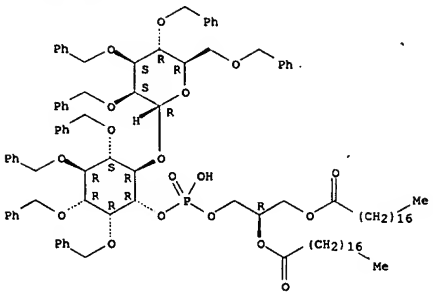
RN 908853-77-0 CAPLUS
CN D-myo-Inositol, 2,3,4,5-tetrakis-O-(phenylmethyl)-6-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, hydrogen (2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl phosphate, compd. with N,N-diethylethanamine (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 908853-76-9
CMF C107 H145 O18 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 4 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

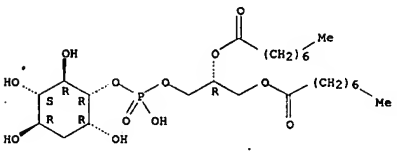
L31 ANSWER 5 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:476267 CAPLUS
DOCUMENT NUMBER: 145:167472
TITLE: Streamlined Synthesis of Phosphatidylinositol (PI), PI3P, PI3,5P2, and Deoxygenated Analogues as Potential
Biological Probes
AUTHOR(S): Xu, Yingju; Sculimbrene, Bianca R.; Miller, Scott J.
CORPORATE SOURCE: Department of Chemistry, Boston College, Chestnut Hill, MA, 02467, USA
SOURCE: Journal of Organic Chemistry (2006), 71(13), 4919-4928
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:167472

AB Highly direct total syntheses of phosphatidylinositol (PI), phosphatidylinositol-3-phosphate (PI3P), phosphatidylinositol-3,5-bis-phosphate (PI3,5P2), and a range of deoxygenated versions are reported. Each synthesis is carried out to deliver the target in optically pure form. The key step for each synthesis is a catalytic asym. phosphorylation reaction that affects de-symmetrization of an appropriate myo-inositol precursor. Elaboration to each target compound is then carried out employing a diversity-oriented strategy from the common precursors. In addition to three natural products, several addnl. streamlined total syntheses of deoxygenated PI analogs are reported. These syntheses set the stage for high-precision biol. investigations of polar headgroup/biol. target interactions of these membrane-associated signaling mols.

IT 899827-42-0P 899827-45-3P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(streamlined synthesis of phosphatidylinositol (PI), PI3P, PI3,5P2 and deoxygenated analogs as potential biol. probes)
RN 899827-42-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

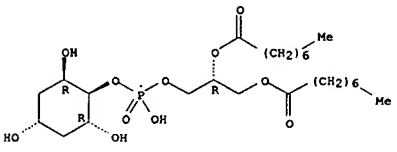
L31 ANSWER 5 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 899827-45-3 CAPLUS
CN Octanoic acid, (1R)-1-[[[hydroxy[[(1α,2R,4β,6R)-2,4,6-trihydroxycyclohexyl]oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

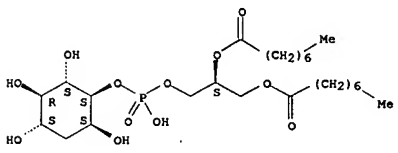


● Na

IT 899827-51-1P 900159-90-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(streamlined synthesis of phosphatidylinositol (PI), PI3P, PI3,5P2 and deoxygenated analogs as potential biol. probes)
RN 899827-51-1 CAPLUS
CN D-chiro-Inositol, 1-deoxy-, 5-[(2S)-2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

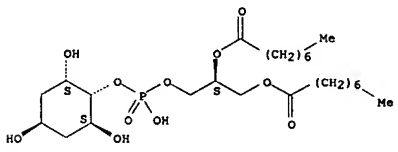
L31 ANSWER 5 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 900159-90-2 CAPLUS
CN Octanoic acid, (1S)-1-[[[hydroxy[[(1α,2S,4β,6S)-2,4,6-trihydroxycyclohexyl]oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



● Na

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 6 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:239690 CAPLUS
DOCUMENT NUMBER: 145:477
TITLE: Spectrum of activity and molecular correlates of response to phosphatidylinositol ether lipid analogues, novel lipid-based inhibitors of Akt
AUTHOR(S): Gills, Joell J.; Holbeck, Susan; Hollingshead, Melinda; Hewitt, Stephen M.; Kozikowski, Alan P.; Dennis, Phillip A.
CORPORATE SOURCE: Medical Oncology Branch and Tissue Array Research Program, Laboratory of Pathology, Center for Cancer Research, National Cancer Institute, Bethesda, MD, USA
SOURCE: Molecular Cancer Therapeutics (2006), 5(3), 713-722 CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

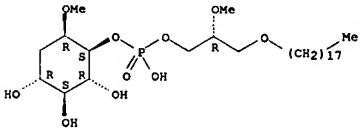
AB The serine/threonine kinase Akt is a promising target in cancer. We previously identified five phosphatidylinositol ether lipid analogs (PIA) that inhibited Akt activation and selectively killed lung and breast cancer cells with high levels of Akt activity. To assess the spectrum of activity in other cell types and to compare PIAs with other inhibitors of the phosphatidylinositol 3-kinase (PI3K)/Akt/mammalian target of rapamycin (mTOR) pathway, we compared growth inhibition by PIAs against the PI3K inhibitors LY294002 and wortmannin and the mTOR inhibitor rapamycin in the NCI60 cell line panel. Although each of these compds. inhibited the growth of all the cell lines, distinct patterns were observed The PIAs were the least potent but the most cytotoxic. The broad spectrum of activity of PIAs was confirmed in vivo in hollow fiber assays. The response to PIAs was significantly correlated with levels of active but not total Akt in the NCI60, as assessed using COMPARE anal. However, a number of mol. targets were identified whose expression was more highly correlated with sensitivity to PIAs than active Akt. Expression of these mol. targets did not overlap with those that correlated with sensitivity to LY294002, wortmannin, or rapamycin. A COMPARE anal. of the National Cancer Institute chemical screening database revealed that the patterns of activity of PIAs correlated best with patterns of activity of other lipid-based compds. These studies show that although PIAs are widely active in cancer cells, which correlates with the presence of its intended target, active Akt, PIAs are biol. distinct from other known inhibitors of the PI3K/Akt/mTOR pathway.

IT 701976-54-7 701976-55-8 701976-68-3
701976-69-4 701976-70-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phosphatidylinositol ether lipid analogs as inhibitors of Akt in cancer)

RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-

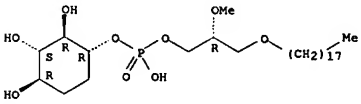
L31 ANSWER 6 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



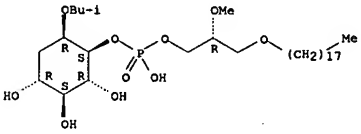
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-68-3 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-(2-methylpropyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

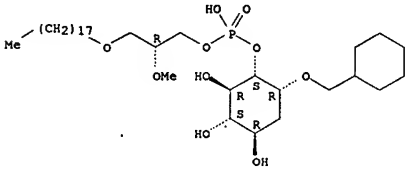
Absolute stereochemistry.



RN 701976-69-4 CAPLUS
CN L-chiro-Inositol, 1-O-(cyclohexylmethyl)-6-deoxy-, 2-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

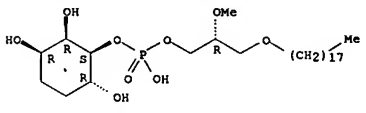
Absolute stereochemistry.

L31 ANSWER 6 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 7 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:167377 CAPLUS
DOCUMENT NUMBER: 144:249992
TITLE: Self-renewal and differentiation in human embryonic stem cells in the presence of PI3-kinase pathway inhibitor and TGFβ family member
INVENTOR(S): Dalton, Stephen; Sheppard, Allan; Jones, Karen; Baetge, E. Edward; D'Amour, Kevin A.; Agulnick, Alan D.
PATENT ASSIGNEE(S): University of Georgia Research Foundation, Inc., USA; Cythera, Inc.
SOURCE: PCT Int. Appl., 61 pp. CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2006020919 | A2 | 20060223 | WO 2005-US28829 | 20050815 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2005272681 | A1 | 20060223 | AU 2005-272681 | 20050815 |
| CA 2576872 | A1 | 20060223 | CA 2005-2576872 | 20050815 |
| EP 1791952 | A2 | 20070606 | EP 2005-790287 | 20050815 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU | | | | |

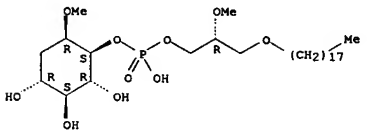
PRIORITY APPLN. INFO.: US 2004-601664P P 20040813
WO 2005-US28829 W 20050815

AB The present invention provides compns. and methods for the production of differentiated mammalian cells (e.g., human cells). More particularly, the present invention provides cellular differentiation methods employing culturing the cells on a feeder layer or under feeder-free conditions in cell culture and further contacting the cells with an inhibitor of the PI3-kinase pathway (e.g., rapamycin) and a member of the TGFβ family (e.g., activin A) for the generation of differentiated mammalian cells from pluripotent mammalian stem cells. The differentiated cell is selected from the group consisting of a mesendodermal cell, a mesodermal cell, and an endodermal cell (preferably, an endodermal cell).

IT 701976-54-7, Akt inhibitor II
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(PI3 inhibitor SH5; self-renewal and differentiation in human embryonic stem cells in presence of PI3-kinase pathway inhibitor and TGFβ family member)

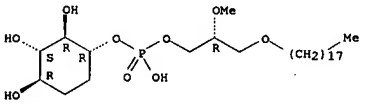
L31 ANSWER 7 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

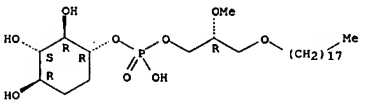


IT 701976-55-8, Akt inhibitor III
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(PI3 inhibitor SH6; self-renewal and differentiation in human embryonic
stem cells in presence of PI3-kinase pathway inhibitor and TGFβ family member)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 8 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 8 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:65453 CAPLUS
DOCUMENT NUMBER: 145:305797
TITLE: Bcl-2 attenuates anticancer agents-induced apoptosis by sustained activation of Akt/protein kinase B in U937 cells
AUTHOR(S): Woo, K. J.; Yoo, Y. H.; Park, J.-W.; Kwon, T. K.
CORPORATE SOURCE: Department of Immunology, School of Medicine, Keimyung
University, Taegu, 700-712, S. Korea
SOURCE: Apoptosis (2005), 10(6), 1333-1343
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aberrant overexpression of antiapoptotic members of the Bcl-2 protein family contributes to resistance to anticancer therapeutic drugs. Thus, this protein represent attractive target for novel anticancer agents. In the present study, we determined the effect of the anti-apoptosis protein Bcl-2
on caspase-3 activation, PLC-γ1 degradation and Akt activation during the various anticancer agents-induced apoptosis. Treatment with chrysin for 12 h produced morphol. features of apoptosis in U937 cells, which was associated with caspase-3 activation and PLC-γ1 degradation Induction of
apoptosis was also accompanied by down-regulation of XIAP and inactivation
of Akt. Chrysin-induced caspase-3 activation, PLC-γ1 degradation and apoptosis were significantly attenuated in Bcl-2 overexpressing U937/Bcl-2
cells. Ectopic expression of Bcl-2 appeared to inhibit ceramide-, and Akt
specific inhibitor (SH-6)-induced apoptosis by sustained Akt activation. Thus, our findings imply that some of the biol. functions of Bcl-2 may be attributed to their ability to inhibit anticancer agents-induced apoptosis
through the sustained Akt activation.
IT 701976-55-8, SH 6 (enzyme inhibitor)
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(induction of apoptosis was also accompanied by down-regulation of XIAP
and inactivation of Akt)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 9 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:984081 CAPLUS
DOCUMENT NUMBER: 143:300314
TITLE: Sequences of novel human APO2L and IL-24 splice variant polypeptides, polynucleotides, and methods of their use in cancer therapy
INVENTOR(S): Wang, Yan; Collins, Amy L. Tsui; Hestir, Kevin; Lee, Ernestine; Halenbeck, Robert Forgan; Bosch, Elizabeth;
Linnemann, Thomas; Williams, Lewis T.
PATENT ASSIGNEE(S): Five Prime Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005082934 | A2 | 20050909 | WO 2005-US5221 | 20050218 |
| WO 2005082934 | A3 | 20051215 | | |

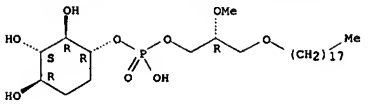
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| PRIORITY APPLN. INFO.: | | |
|---|---|---|
| US 2004-546385P | P | 20040220 |
| US 2005-647013P | P | 20050127 |
| US 2005-654229P | P | 20050218 |

AB The present invention discloses newly identified human interleukin 24 and APO2L splice variant mols., their polypeptide sequences, and the polynucleotides encoding the polypeptide sequences. Also provided is a procedure for producing such polypeptides by recombinant techniques employing, for example, vectors and host cells, and, for example, heterologous secretory leader sequences. Also disclosed are methods for using such polypeptides and modulators thereof for the treatment of diseases, including cancer, immune diseases, infectious diseases, and ischemic diseases.
IT 701976-55-8, SH 6
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sequences of novel human APO2L and IL-24 splice variant polypeptides, polynucleotides, and methods of their use in cancer therapy)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 9 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L31 ANSWER 10 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:979659 CAPLUS
DOCUMENT NUMBER: 143:279354
TITLE: Lysophosphatidic acid (LPA) derivative modulators of LPA signaling, and therapeutic use
INVENTOR(S): Hasegawa, Yutaka; Mills, Gordon B.
PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
SOURCE: PCT Int. Appl., 160 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005082914 | A2 | 20050909 | WO 2004-US42395 | 20041215 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-546601P P 20040220
US 2004-555235P P 20040322

OTHER SOURCE(S): MARPAT 143:279354

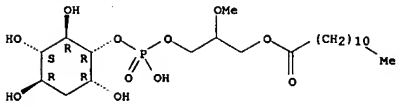
AB The invention provides LPA derivative compds. and pharmaceutical compns. involved in LPA signaling and methods of treating a disease (e.g. cancer) using compds. and compns. of the invention.

IT 864144-62-7 864144-63-8 864144-64-9
864144-65-0 864144-66-1 864144-67-2
864144-68-3 864144-69-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lysophosphatidic acid (LPA) derivative modulators of LPA signaling, and therapeutic use)

RN 864144-62-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[(1-oxododecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

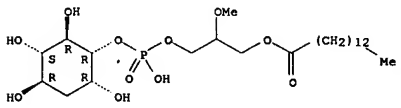
Absolute stereochemistry.

L31 ANSWER 10 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



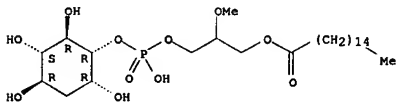
RN 864144-63-8 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[(1-oxotetradecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



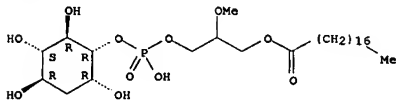
RN 864144-64-9 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864144-65-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

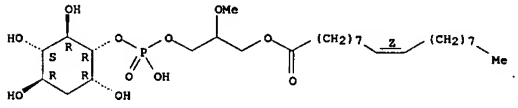
Absolute stereochemistry.



RN 864144-66-1 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[[(9Z)-1-oxo-9-octadecenyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L31 ANSWER 10 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

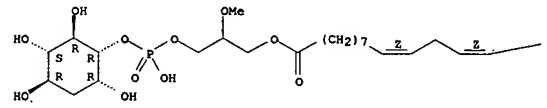
Absolute stereochemistry.
Double bond geometry as shown.



RN 864144-67-2 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[[(9Z,12Z)-1-oxo-9,12-octadecadienyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

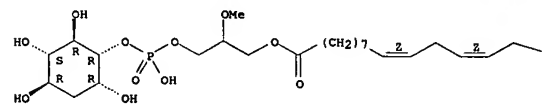


PAGE 1-B

RN 864144-68-3 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[[(9Z,12Z,15Z)-1-oxo-9,12,15-octadecatrienyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



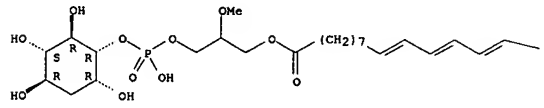
L31 ANSWER 10 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

RN 864144-69-4 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[2-methoxy-3-[(1-oxo-9,11,13-octadecatrienyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B

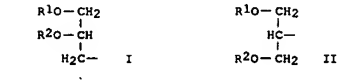
Bu-n

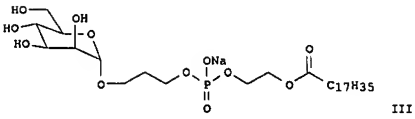
L31 ANSWER 11 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:472171 CAPLUS
DOCUMENT NUMBER: 143:7937
TITLE: Preparation of acyl glycerol phosphatidylinositol manno-oligosaccharides as anti-inflammatory agents
INVENTOR(S): Singh-Gill, Gurmit; Larsen, David Samuel; Jones, Jeremy David; Severn, Wayne Bruce; Harper, Jacquie Lucille
PATENT ASSIGNEE(S): The Malaghan Institute of Medical Research, N. Z.; University of Otago; Agresearch Limited
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005049631 | A1 | 20050602 | WO 2004-NZ293 | 20041118 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| NZ 529603 | A | 20031219 | NZ 2003-529603 | 20031118 |
| PRIORITY APPLN. INFO.: | | | NZ 2003-529603 A | 20031118 |
| | | | NZ 2004-533245 A | 20040531 |

OTHER SOURCE(S): CASREACT 143:7937; MARPAT 143:7937
GI

L31 ANSWER 11 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)





III

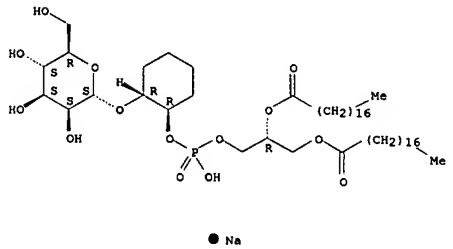
AB The present invention is directed to synthetic acyl glycerol phosphatidylinositol manno-oligosaccharides having the formula A-B-E-D, wherein A is R, glyceride I and II; R is H, alkyl, acyl; B is phosphate, phosphonate, sulfonate, carbamate, phosphono-thionate; E is a spacer or linker (CH2)n, (CH2)2-(OCH2CH2)n, cyclohexyl, CHR3CHR4; R3 and R4 are independently H, CH2OH, CH2, alditol residue; n is 1-40; D comprises at least one sugar moiety selected from the group comprising D-mannose, D-galactose, D-glucose, D-glucosamine, N-acetylglucosamine, and 6-deoxy-L-mannose, wherein when D is more than one sugar moiety, the sugar moiety may comprise a single chain of the same or different sugar moieties, or may comprise two or more sep. sugar moieties or chains of sugar moieties attached to E at different sites; with the proviso that when E is -(CH2)n- wherein n = 2 to 16, B is phosphate and D is a monosaccharide or an oligosaccharide, R1 and R2 of A are not both alkyl.is biol. activity similar to PIM (acyl glycerol phosphatidylinositol manno-oligosaccharide) activity, for use in the treatment and prevention of inflammatory or immune cell mediated diseases or disorders. The disease or disorder is elected from the group comprising asthma, allergic rhinitis, dermatitis, psoriasis, inflammatory bowel disease including Crohn's disease and ulcerative colitis, rheumatoid arthritis, multiple sclerosis, diabetes, systemic lupus erythmatosis and atherosclerosis. Thus, III was prepared and tested in mice as anti-inflammatory agent.

IT 852395-76-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acyl glycerol phosphatidylinositol manno-oligosaccharides as antiinflammatory agents)

RN 852395-76-7 CAPLUS
CN α-D-Mannopyranoside, (1R,2R)-2-[[[(2R)-2,3-bis[(1-oxooctadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]cyclohexyl, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L31 ANSWER 11 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L31 ANSWER 12 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:451176 CAPLUS
DOCUMENT NUMBER: 143:1222
TITLE: Modulating substances of the nitric oxide-cyclic guanosine 3',5'-monophosphate signaling pathway for the treatment of dental disorders
INVENTOR(S): Baumann, Michael; Bloch, Wilhelm; Korkmaz, Yueksel
PATENT ASSIGNEE(S): Cell Center Cologne G.m.b.H., Germany
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005046660 | A1 | 20050526 | WO 2004-EP12935 | 20041115 |

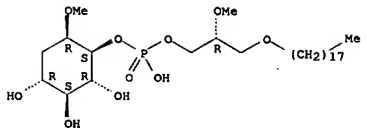
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2003-26132 A 20031113

AB The use of a modulating substance of the nitric oxide (NO)-cyclic guanosine 3',5'-monophosphate (cGMP) signaling pathway for the preparation of a pharmaceutical composition for the prevention and/or treatment of a dental disorder in a mammal is disclosed. Furthermore, pharmaceutical compns. comprising a modulating substance of the NO-cGMP signaling pathway as well as methods for treating a dental disorder are provided.
IT 701976-54-7, SH 5 701976-55-8, SH 6
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(modulating substances of the nitric oxide-cyclic GMP signaling pathway for the treatment of dental disorders)
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

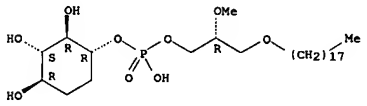
Absolute stereochemistry.

L31 ANSWER 12 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.

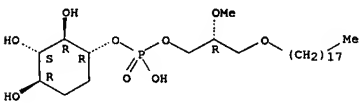


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 13 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:339752 CAPLUS
DOCUMENT NUMBER: 143:109462
TITLE: Fenofibrate induces apoptotic injury in cultured human hepatocytes by inhibiting phosphorylation of Akt
AUTHOR(S): Kubota, T.; Yano, T.; Fujisaki, K.; Itoh, Y.; Oishi, R.
CORPORATE SOURCE: Department of Pharmacy, Kyushu University Hospital, Higashi-ku, Fukuoka, 812-8582, Japan
SOURCE: Apoptosis (2005), 10(2), 349-358
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fibric acid derivs. have a potent and effective lipid-lowering action, however, the use of these compds. is sometimes limited due to the occurrence of hepatic injury. In the present study, we characterized cell injury induced by fenofibrate in cultured human hepatocytes. Fenofibrate caused a loss of cell viability and nuclear damage as assessed by terminal deoxynucleotidyl transferase-mediated dUTP nick end-labeling or by DNA electrophoresis, in which caspase activation is involved. The cell injury was accompanied by the shrinkage and the translocation of phosphatidyl serine from inner membrane to the outer membrane as determined by annexin V stain. The mRNA expression for bcl-2 was reduced by fenofibrate. An immunofluorescent stain with antiserum raised against phosphorylated Akt revealed that fenofibrate inhibited insulin-stimulated phosphorylation of Akt. Like fenofibrate, several compds. that inhibit the phosphorylation of Akt, including wortmannin, SH-6 and a high concentration (100 μM) of SB203580, reduced the viability of cultured human hepatocytes. Both nuclear damage and cell injury induced by fenofibrate were reversed by insulin in a concentration-dependent manner. In contrast, bezafibrate or 8(S)-hydroxyeicosatetraenoic acid had no hepatotoxic action. These findings suggest that fenofibrate causes caspase-dependent apoptosis in human hepatocytes by inhibiting phosphorylation of Akt, in which PPARα is not involved.
IT 701976-55-8
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(fenofibrate caused caspase-dependent apoptosis in human hepatocytes by inhibiting phosphorylation of Akt, in which peroxisome proliferator-activated receptor-α was not involved)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



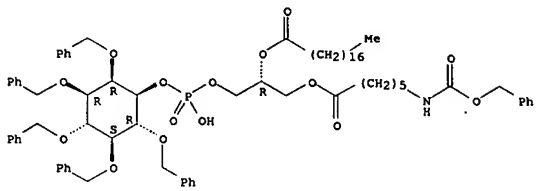
L31 ANSWER 13 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 14 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:246004 CAPLUS
DOCUMENT NUMBER: 142:477538
TITLE: New fluorescent probes reveal that flippase-mediated flip-flop of phosphatidylinositol across the endoplasmic reticulum membrane does not depend on the stereochemistry of the lipid
AUTHOR(S): Vishwakarma, Ram A.; Vehring, Stefanie; Mehta, Anuradha; Sinha, Archana; Pomorski, Thomas; Herrmann, Andreas; Menon, Anant K.
CORPORATE SOURCE: Bio-Organic Chemistry Laboratory, National Institute of Immunology, New Delhi, 110067, India
SOURCE: Organic & Biomolecular Chemistry (2005), 3(7), 1275-1283
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:477538
AB Glycerophospholipid flip-flop across biogenic membranes such as the endoplasmic reticulum (ER) is a fundamental feature of membrane biogenesis. Flip-flop requires the activity of specific membrane proteins called flippases. These proteins have yet to be identified in biogenic membranes and the mol. basis of their action is unknown. It is generally believed that flippase-facilitated glycerophospholipid flip-flop across the ER is governed by the stereochem. of the glycerolipid, but this important issue has not been resolved. Here the authors investigate whether the ER flippase stereochem. recognizes the glycerophospholipids that it transports. To address this question the authors selected phosphatidylinositol (PI), a biol. important mol. with chiral centers in both its myo-inositol headgroup and its glycerol-lipid tail. The flip-flop of PI across the ER has not been previously reported. The authors synthesized fluorescence-labeled forms of all four diastereoisomers of PI and evaluated their flipping in rat liver ER vesicles, as well as in flippase-containing proteoliposomes reconstituted from a detergent extract of ER. The results show that the flippase is able to translocate all four PI isomers and that both glycerol isomers of PI flip-flop across the ER membrane at rates similar to that measured for fluorescence-labeled phosphatidylcholine. The authors' data have important implications for recent hypotheses concerning the evolution of distinct homochiral glycerophospholipid membranes during the speciation of archaea and bacteria/eukarya from a common cellular ancestor.
IT 852066-08-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phosphatidylinositol-based fluorescent probes preparation and use in anal. of stereochem. of flippase-mediated flip-flop of phosphatidylinositol across endoplasmic reticulum membrane)
RN 852066-08-1 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2-[(1-oxooctadecyl)oxy]-3-[[1-oxo-6-[[(phenylmethoxy)carbonyl]amino]hexyl]oxy]pr

L31 ANSWER 14 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
opyl hydrogen phosphate (9CI) (CA INDEX NAME)

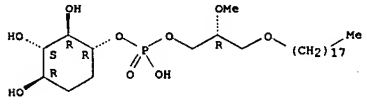
Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 15 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:141521 CAPLUS
DOCUMENT NUMBER: 142:423232
TITLE: TRAIL-induced apoptosis in gliomas is enhanced by Akt-inhibition and is independent of JNK activation
AUTHOR(S): Puduvalli, V. K.; Sampath, D.; Bruner, J. M.; Nangia, J.; Xu, R.; Kyritsis, A. P.
CORPORATE SOURCE: Departments of Neuro-Oncology, The University of Texas M. D. Anderson Cancer Center, Houston, TX, 77030, USA
SOURCE: Apoptosis (2005), 10(1), 233-243
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Patients with malignant gliomas have a poor prognosis and new treatment paradigms are needed against this disease. TRAIL/Apo2L selectively induces apoptosis in malignant cells sparing normal cells and is hence of interest as a potential therapeutic agent against gliomas. To determine the factors that modulate sensitivity to TRAIL, we examined the differences in TRAIL-activated signaling pathways in glioma cells with variable sensitivities to the agent. Apoptosis in response to TRAIL was unrelated to DR5 expression or endogenous p53 status in a panel of 8 glioma cell lines. TRAIL activated the extrinsic (cleavage of caspase-8, caspase-3 and PARP) and mitochondrial apoptotic pathways and reduced FLIP levels. It also induced caspase-dependent JNK activation, which did not influence TRAIL-induced apoptosis. Because the pro-survival PI3K/Akt pathway is highly relevant to gliomas, we assessed whether Akt could protect against TRAIL-induced apoptosis. Pretreatment with SH-6, a novel Akt inhibitor, enhanced TRAIL-induced apoptosis, suggesting a protective role for Akt. Conversely, TRAIL induced caspase-dependent cleavage of Akt neutralizing its anti-apoptotic effects. These results demonstrate that TRAIL-induced apoptosis in gliomas involves both activation of death pathways and downregulation of survival pathways. Addnl. studies are warranted to determine the therapeutic potential of TRAIL against gliomas.
IT 701976-55-8, SH 6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Akt inhibitor SH-6 enhanced TNF-related apoptosis inducing ligand induced apoptosis in human malignant glioma D54MG, U251MG, U87MG, U343, U373, A172, LN229, T98G cells)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 15 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

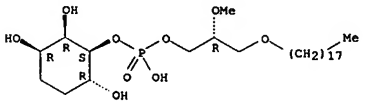
L31 ANSWER 16 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:133799 CAPLUS
DOCUMENT NUMBER: 142:423229
TITLE: Activated forms of H-RAS and K-RAS differentially regulate membrane association of PI3K, PDK-1, and AKT and the effect of therapeutic kinase inhibitors on cell survival
AUTHOR(S): Caron, Ruben W.; Yacoub, Adly; Li, Min; Zhu, Xiaoyu; Mitchell, Clint; Hong, Young; Hawkins, William; Sasazuki, Takehiko; Shirasawa, Senji; Kozikowski, Alan P.; Dennis, Philip A.; Hagan, Michael P.; Grant, Steven; Dent, Paul
CORPORATE SOURCE: Departments of Radiation Oncology and Hematology/Oncology, Virginia Commonwealth University, Richmond, VA, USA
SOURCE: Molecular Cancer Therapeutics (2005), 4(2), 257-270 CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The abilities of mutated active RAS proteins to modulate cell survival following exposure to ionizing radiation and small mol. kinase inhibitors were examined Homologous recombination in HCT116 cells to delete the single allele of K-RAS D13 resulted in a cell line that exhibited an .apprx.75% reduction in basal extracellular signal-regulated kinase 1/2, AKT, and c-jun-NH2-kinase 1/2 activity. Transfection of cells lacking K-RAS D13 with H-RAS V12 restored extracellular signal-regulated kinase 1/2 and AKT activity to basal levels but did not restore c-jun-NH2-kinase 1/2 phosphorylation. In cells expressing H-RAS V12, radiation caused prolonged intense activation of AKT. Inhibition of H-RAS V12 function, blockade of phosphatidylinositol 3-kinase (PI3K) function using small interfering RNA/small-mol. inhibitors, or expression of dominant-neg. AKT abolished radiation-induced AKT activation, and radiosensitized these cells. Inhibition of PI3K function did not significantly radiosensitize parental HCT116 cells. Inhibitors of the AKT PH domain including perifosine, SH-(5, 23 - 25) and ml-(14 - 16) reduced the plating efficiency of H-RAS V12 cells in a dose-dependent fashion. Inhibition of AKT function using perifosine enhanced radiosensitivity in H-RAS V12 cells, whereas the SH and ml series of AKT PH domain inhibitors failed to promote radiation toxicity. In HCT116 H-RAS V12 cells, PI3K, PDK-1, and AKT were membrane associated, whereas in parental cells expressing K-RAS D13, only PDK-1 was membrane bound. In H-RAS V12 cells, membrane associated PDK-1 was phosphorylated at Y373/376, which was abolished by the Src family kinase inhibitor PP2. Inhibition of PDK-1 function using the PH domain inhibitor OSU-03012 or using PP2 reduced the plating efficiency of H-RAS V12 cells and profoundly increased radiosensitivity. OSU-03012 and PP2 did not radiosensitize and had modest inhibitory effects on plating efficiency in parental cells. A small interfering RNA generated against PDK1 also radiosensitized HCT116 cells expressing H-RAS V12. Collectively, our data argue that mol. inhibition of AKT and PDK-1 signaling enhances the radiosensitivity of HCT116 cells expressing H-RAS V12 but not K-RAS D13. Small-mol. inhibitory agents that blocked stimulated and/or basal PDK-1 and AKT function profoundly reduced HCT116 cell survival but had variable effects at enhancing tumor cell radiosensitivity.

IT 701976-70-7 850894-86-9 850894-87-0
850894-89-2 850894-90-5 850894-91-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(activated forms of H-RAS and K-RAS differentially regulate membrane association of PI3K, PDK-1, and AKT and the effect of therapeutic kinase inhibitors on cell survival)

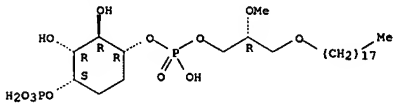
RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



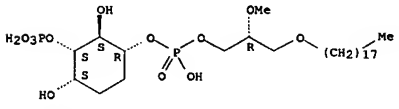
RN 850894-86-9 CAPLUS
CN Phosphoric acid, mono[(1R,2R,3R,4S)-2,3-dihydroxy-4-(phosphonooxy)cyclohexyl] mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



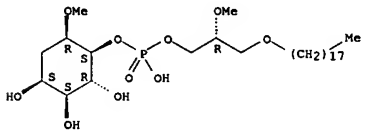
RN 850894-87-0 CAPLUS
CN Phosphoric acid, mono[(1R,2S,3S,4S)-2,4-dihydroxy-3-(phosphonooxy)cyclohexyl] mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



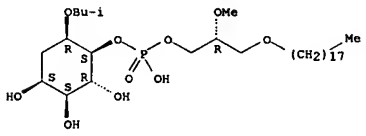
RN 850894-89-2 CAPLUS
CN D-epi-Inositol, 3-deoxy-2-O-methyl-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



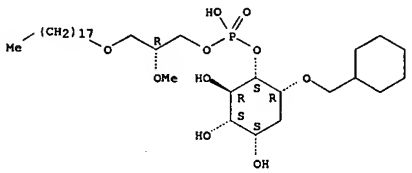
RN 850894-90-5 CAPLUS
CN D-epi-Inositol, 3-deoxy-2-O-(2-methylpropyl)-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850894-91-6 CAPLUS
CN D-epi-Inositol, 2-O-(cyclohexylmethyl)-3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

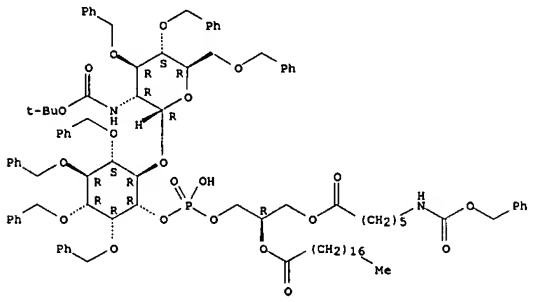
Absolute stereochemistry.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:42067 CAPLUS
DOCUMENT NUMBER: 142:293142
TITLE: Flip-flop of glycosylphosphatidylinositols (GPI's) across the ER
AUTHOR(S): Vishwakarma, Ram A.; Menon, Anant K.
CORPORATE SOURCE: Bio-Organic Chemistry Laboratory, National Institute of Immunology, New Delhi, 110067, India
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (4), 453-455
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:293142
AB The transbilayer flip-flop of early intermediates in the glycosylphosphatidylinositol (GPI) biosynthetic pathway has been demonstrated using novel fluorescent GPI probes and a biochem. reconstitution approach.
IT 847789-93-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(flip-flop of glycosylphosphatidylinositols (GPI's) across the ER)
RN 847789-93-9 CAPLUS
CN D-myo-Inositol, 6-O-[2-deoxy-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2-[(1-oxooctadecyl)oxy]-3-[[1-oxo-6-[[(phenylmethoxy)carbonyl]amino]hexyl]oxy]propyl hydrogen phosphate] (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

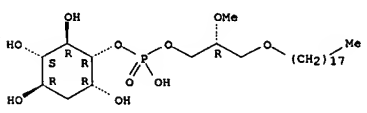


L31 ANSWER 17 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 18 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1087440 CAPLUS
DOCUMENT NUMBER: 142:273578
TITLE: In vivo molecular pharmacology and antitumor activity of the targeted Akt inhibitor PX-316
AUTHOR(S): Meuillet, Emmanuelle J.; Ihle, Nathan; Baker, Amanda F.; Gard, Jaime M.; Stamper, Chelsea; Williams, Ryan; Coon, Amy; Mahadevan, Daruka; George, Benjamin L.; Kirkpatrick, Lynn; Powis, Garth
CORPORATE SOURCE: Arizona Cancer Center, University of Arizona, Tucson, AZ, 85724, USA
SOURCE: Oncology Research (2004), 14(10), 513-527
CODEN: ONREE8; ISSN: 0965-0407
PUBLISHER: Cognizant Communication Corp.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Akt, a serine/threonine kinase that promotes cell survival, is activated by binding of its pleckstrin homol. (PH) domain to membrane phosphatidylinositol (PtdIns)-3-phosphates formed by PtdIns-3-kinase. D-3-Deoxy-phosphatidyl-myo-inositols that cannot be phosphorylated on the 3-position of the myo-inositol group are inhibitors of the Akt PH domain. The most active compound is D-3-deoxy-phosphatidyl-myo-inositol 1-[(R)-2-methoxy-3-octadecyloxypropyl hydrogen phosphate] (PX-316). PX-316 administered i.p. to mice at 150 mg/kg inhibits Akt activation in HT-29 human tumor xenografts up to 78% at 10 h with recovery to 34% at 48 h. Phosphorylation of GSK-3β, a downstream target of Akt, is also inhibited. There is no decrease in PtdIns(3,4,5)-trisphosphate levels by PX-316, showing it is not an inhibitor of PtdIns-3-K in vivo. Gene expression profiling of HT-29 tumor xenografts shows many similarities between the effects of PX-316 and the PtdIns-3-K inhibitor wortmannin, with downregulation of several ribosomal-related genes, while PX-316 uniquely increases the expression of a group of mitochondrial-related genes. PX-316 has antitumor activity against early human MCF-7 breast cancer and HT-29 colon cancer xenografts in mice. PX-316 formulated in 20% hydroxypropyl-β-cyclodextrin for i.v. administration is well tolerated in mice and rats with no hemolysis and no hematol. toxicity. Thus, PX-316 is the lead compound of a new class of potential agents that inhibit Akt survival signaling.
IT 253440-95-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Akt inhibitor PX-316 inhibited phosphorylation of its downstream targets in human HT-29 tumor xenograft in SCID mouse without inhibiting
(ptdIns2)-3-K, showed antitumor activity on human MCF-7, HT-29 xenograft and less toxic in rat, mouse)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

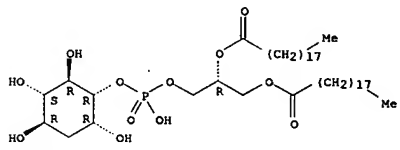
Absolute stereochemistry.



L31 ANSWER 18 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 847147-75-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(PX-315 had less affinity to bind to PH domain of Akt than PX-316 in vitro)
RN 847147-75-5 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxononadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

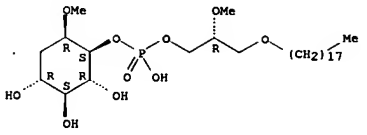
L31 ANSWER 19 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:759995 CAPLUS
DOCUMENT NUMBER: 142:126804
TITLE: Novel 2'-substituted, 3'-deoxy-phosphatidyl-myo-inositol analogues reduce drug resistance in human leukaemia cell lines with an activated phosphoinositide 3-kinase/Akt pathway
AUTHOR(S): Tabellini, Giovanna; Tazzari, Pier Luigi; Bortul, Roberta; Billi, Anna Maria; Conte, Roberto; Manzoli, Lucia; Cocco, Lucio; Martelli, Alberto M.
CORPORATE SOURCE: Dipartimento di Scienze Anatomiche Umane e Fisiopatologia dell'Apparato Locomotore, Sezione di Anatomia, Cell Signaling Laboratory, Universita di Bologna, Bologna, Italy
SOURCE: British Journal of Haematology (2004), 126(4), 574-582
CODEN: BJHEAL; ISSN: 0007-1048
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Activation of the phosphoinositide 3-kinase (PI3-K)/Akt signalling pathway has been linked with resistance to chemotherapeutic drugs, and its down-regulation, by means of pharmacol. inhibitors of PI3-K, considerably lowers resistance to various types of therapy in cell lines derived from solid tumors. Recently, a new class of Akt inhibitors, referred to as phosphatidylinositol ether lipids (PIAs), have been synthesized. We tested whether two new PIAs could lower the sensitivity threshold to chemotherapeutic drugs of human leukemia cell lines with an activated PI3-K/Akt network. We used HL60AR (for apoptosis resistant), K562 and U937 cells. The two pharmacol. inhibitors, used at 5 μmol/l, down-regulated Akt kinase activity and phosphorylation. Neither of the two chems. affected the activity of other signalling proteins in the Akt pathway, such as phosphoinositide-dependent protein kinase-1 or PTEN. When employed at 5 μmol/l, the Akt inhibitors markedly reduced the resistance of the leukemic cell lines to etoposide or cytarabine. Remarkably, a 5 μmol/l concentration of the inhibitors did not neg. affect the survival rate of human cord blood CD34+ cells. Overall, our results indicate that new selective Akt pharmacol. inhibitors might be used in the future for overcoming Akt-mediated resistance to therapeutic treatments of acute leukemia cells.

IT 701976-54-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SH-5; Akt inhibitors SH-5 and SH-6 decreased Akt kinase activity, phosphorylation, reduced leukemic cell resistance to etoposide and cytarabine but gave no effect on PTEN and CB CD34+ survival rate in HL60AR, HL60PT, K562 and U937 cell line)
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

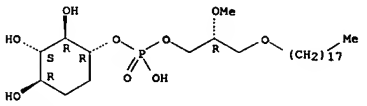
Absolute stereochemistry.

L31 ANSWER 19 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 701976-55-8, D-2,3-Dideoxy-2-myo-inositol 1-[(R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate]
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SH-6; Akt inhibitors SH-5 and SH-6 decreased Akt kinase activity, phosphorylation, reduced leukemic cell resistance to etoposide and cytarabine but gave no effect on PTEN and CB CD34+ survival rate in HL60AR, HL60PT, K562 and U937 cell line)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 20 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:412760 CAPLUS
DOCUMENT NUMBER: 140:417918
TITLE: Hydroxyflutamide induced pathways related to androgen receptor negative prostate cancer cells
INVENTOR(S): Chang, Chawnshang; Lee, Yi-fen; Lin, Wen-jye
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004041185 | A2 | 20040521 | WO 2003-US34636 | 20031031 |
| WO 2004041185 | A3 | 20040826 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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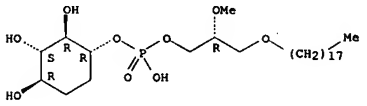
|---|---|---|---|---|---|
| AU 2003287366 | A1 | 20040607 | AU 2003-287366 | | 20031031 |
| US 2006270643 | A1 | 20061130 | US 2006-533037 | | 20060331 |
| PRIORITY APPLN. INFO.: | | | US 2002-423340P | P | 20021031 |
| | | | WO 2003-US34636 | W | 20031031 |

AB Disclosed are compns. and methods for reducing androgen receptor dependent cancer cell proliferation. To overcome the problems associated with androgen ablation treatment and more specifically antiandrogen withdrawal syndrome, disclosed herein are compns. comprising combination therapies for the treatment of prostate cancer based on the links in prostate cancer and the pathways disclosed herein. Thus disclosed are compns. comprising an inhibitor of the MAP kinase or MEK pathway signal transduction pathway and an antiandrogen, such as flutamide or hydroxyflutamide. Also, specifically disclosed are compns. comprising an antiandrogen and an anti-phosphatidylinositol 3-kinase (PI3K)/Akt kinase inhibitor.

IT 701976-55-8, SH 6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hydroxyflutamide induced pathways related to androgen receptor neg. prostate cancer cells in relation to treatment with antiandrogens and kinase pathway inhibitors and drug screening)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

L31 ANSWER 20 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.



L31 ANSWER 21 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:403059 CAPLUS
DOCUMENT NUMBER: 140:391439
TITLE: Preparation of inositolphospholipids and their structural and stereochemistry analogs via coupling reaction of inositols with glycerophospholpids
INVENTOR(S): Aneja, Rajindra
PATENT ASSIGNEE(S): Nutrimed Biotech, USA
SOURCE: U.S., 13 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

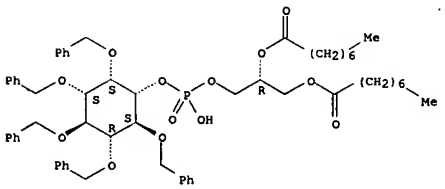
| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| US 6737536 | B1 | 20040518 | US 2002-67648 | | 20020204 |
| PRIORITY APPLN. INFO.: | | | US 2001-266433P | P | 20010205 |

AB This invention relates to inositolphospholipids, particularly to synthetic phosphatidyl-myo-inositols (PtdIns), ceramide-phosphoinositols (CerPhosIns) and their structural and stereochem. analogs 1D-1-(1-fattyacyl1-2-fattyacyl2-sn-glycero-3-phospho)-myo-inositol; 1D-1-(3-fattyacyl1-2-fattyacyl2-sn-glycero-1-phospho)-myo-inositol; 1L-1-(1-fattyacyl1-2-fattyacyl2-sn-glycero-3-phospho)-myo-inositol; 1L-1-(3-fattyacyl1-2-fattyacyl2-sn-glycero-1-phospho)-myo-inositol; wherein fattyacyl1 and fattyacyl2 are identical or non-identical. The invention specifically provides a novel approach to synthesis of inositolphospholipids which is suitable for laboratory scale preparation as well as for large scale industrial production The synthetic approach is applicable equally well for the preparation of inositolphospholipids carrying saturated lipid chains, unsatd. lipid chains with one or more double or triple bonds, chains with hydroxyl, amino and other functional groups, or combinations of these. In addition, it provides novel high purity diastereomer mol. species of inositolphospholipids that have unequivocally defined structure and absolute stereochem. in both the myo-inositol and the glycerol residues and are obtainable only by the present new approach. The invention further provides methods for characterizing and using these high purity diastereomeric compds. Thus, 1L-1-(1,2-dioctanoyl-sn-glycero-3-phospho)-myo-inositol was prepared via coupling of 1,2-dioctanoyl-sn-glycero-3-phosphoric acid and 1D-2,3,4,5,6-penta-O-benzyl-myo-inositol.

IT 264125-32-8P 686285-04-1P 686752-25-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of inositolphospholipids and their structural and stereochem.
analogs via coupling reaction of inositols with glycerophospholpids)

RN 264125-32-8 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-

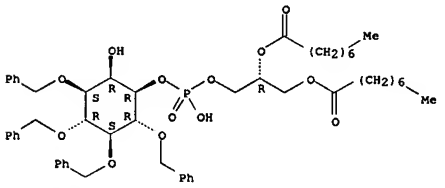
L31 ANSWER 21 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 686285-05-2P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of inositolphospholipids and their structural and stereochem.
analogs via coupling reaction of inositols with glycerophospholpids)

RN 686285-05-2 CAPLUS
CN D-myo-Inositol, 3,4,5,6-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



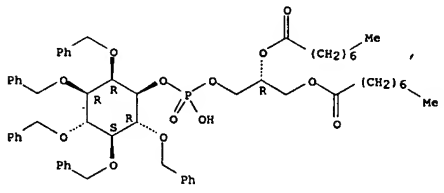
IT 264125-33-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of inositolphospholipids and their structural and stereochem.
analogs via coupling reaction of inositols with glycerophospholpids)

RN 264125-33-9 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

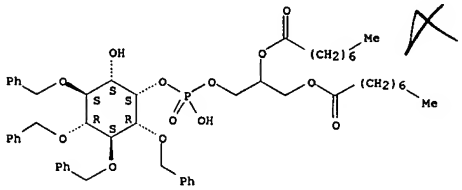
L31 ANSWER 21 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
oxooctyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 686285-04-1 CAPLUS
CN myo-Inositol, 1,4,5,6-tetrakis-O-(phenylmethyl)-, 2-[2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

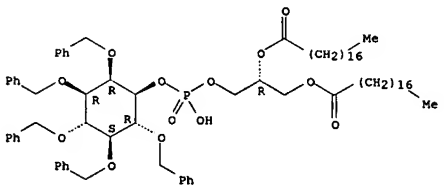
Relative stereochemistry.



RN 686752-25-0 CAPLUS
CN D-myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L31 ANSWER 21 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 22 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:346323 CAPLUS
DOCUMENT NUMBER: 141:89302
TITLE: The synthesis of some deoxygenated analogues of early intermediates in the biosynthesis of glycosylphosphatidylinositol (GPI) membrane anchors
AUTHOR(S): Dix, Alexander P.; Borissow, Charles N.; Ferguson, Michael A. J.; Brimacombe, John S.
CORPORATE SOURCE: School of Life Sciences (Chemistry), University of Dundee, Dundee, DD1 4HN, UK
SOURCE: Carbohydrate Research (2004), 339(7), 1263-1277
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:89302

AB Syntheses are described of 2-azido-4,6-di-O-benzyl-2,3-dideoxy-D-ribo-hexopyranosyl fluoride, 6-O-acetyl-2-azido-3-O-benzyl-2,4-dideoxy-D-xylo-hexopyranosyl fluoride and 2-azido-3,4-di-O-benzyl-2,6-dideoxy-D-glucopyranosyl fluoride. These glycosyl donors were coupled with the acceptor 1d-2,3,4,5-tetra-O-benzyl-1-O-(4-methoxybenzyl)-myo-inositol and the α-coupled products were transformed into α-D-3dGlcpN-PI, α-D-4dGlcpN-PI and α-D-6dGlcpN-PI by way of the H-phosphonate route. Brief mention is made of the biol. evaluation of these deoxy-sugar analogs and their N-acetylated forms as candidate substrate/inhibitors of the N-deacetylase and α-(1→4)-D-mannosyltransferase activities present in trypanosomal and HeLa (human) cell-free system.

IT 324739-91-5P 714957-28-5P 714957-39-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of deoxygenated glycosylphosphatidylinositol membrane anchors analogs and their inhibition of N-deacetylase and α-(1→4)-D-mannosyltransferase in trypanosomal and HeLa cells)

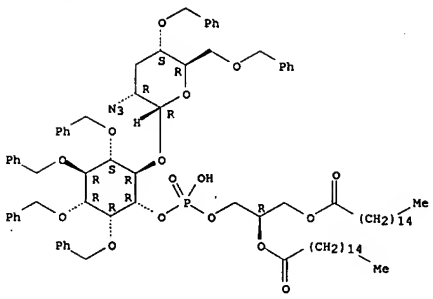
RN 324739-91-5 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2,3-dideoxy-4,6-bis-O-(phenylmethyl)-α-D-ribo-hexopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 324739-90-4
CMF C89 H124 N3 O16 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 22 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

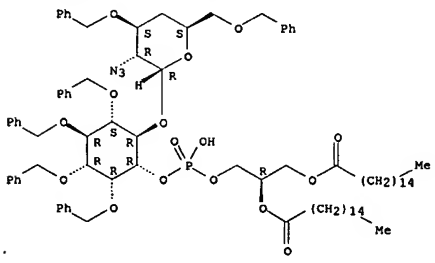
RN 714957-28-5 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2,4-dideoxy-3,6-bis-O-(phenylmethyl)-α-D-xylo-hexopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 714957-27-4
CMF C89 H124 N3 O16 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 22 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N



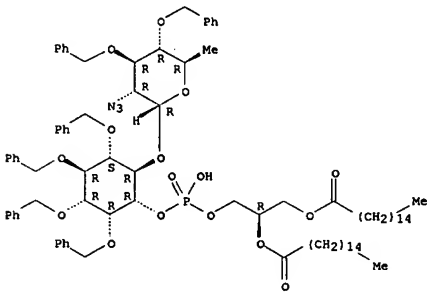
RN 714957-39-8 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2,6-dideoxy-3,4-bis-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 714957-38-7
CMF C89 H124 N3 O16 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 22 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 23 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:309668 CAPLUS
DOCUMENT NUMBER: 141:33428
TITLE: Preferential Inhibition of Akt and Killing of Akt-Dependent Cancer Cells by Rationally Designed Phosphatidylinositol Ether Lipid Analogues
AUTHOR(S): Castillo, S. Sianna; Brognard, John; Petukhov, Pavel A.; Zhang, Chunyu; Tsurutani, Junji; Granville, Courtney A.; Li, Min; Jung, Michael; West, Kip A.; Gills, Joell G.; Kozikowski, Alan P.; Dennis, Phillip A.
CORPORATE SOURCE: Center for Cancer Research, Cancer Therapeutics Branch, National Cancer Institute, Bethesda, MD, USA
SOURCE: Cancer Research (2004), 64(8), 2782-2792
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

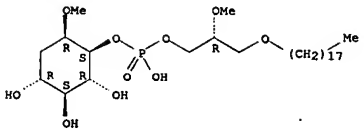
AB Activation of the PI3k/Akt pathway controls key cellular processes and contributes to tumorigenesis in vivo, but investigation of the PI3k/Akt pathway has been limited by the lack of specific inhibitors directed against Akt. To develop Akt inhibitors, we used mol. modeling of the pleckstrin homol. (PH) domain of Akt to guide synthesis of structurally modified phosphatidylinositol ether lipid analogs (PIAs). Here, we characterize the biochem. and cellular effects of PIAs. Of 24 compds. tested, five PIAs with modifications at two sites on the inositol ring inhibited Akt with IC50s < 5 μM. Mol. modeling identified putative interactions of PIAs with the phosphoinositide-binding site in the PH domain of Akt, and growth factor-induced translocation of Akt to the plasma membrane was inhibited by PIA administration. Inhibition of Akt occurred rapidly and was maintained for hours. PIAs decreased phosphorylation of many downstream targets of Akt without affecting upstream kinases, such as PI3k or phosphoinositide-dependent kinase-1, or members of other kinase pathways such as extracellular signal-regulated kinase. Importantly, PIAs increased apoptosis 20 - 30-fold in cancer cell lines with high levels of endogenous Akt activity but only 4 - 5-fold in cancer cell lines with low levels of Akt activity. These studies identify PIAs as effective Akt inhibitors, and provide proof of principle for targeting the PH domain of Akt.

IT 701976-54-7 701976-55-8 701976-57-0 701976-59-2 701976-62-7 701976-65-0 701976-67-2 701976-68-3 701976-69-4 701976-70-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preferential inhibition of Akt and killing of Akt-dependent cancer cells by rationally designed phosphatidylinositol ether lipid analogs)

RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

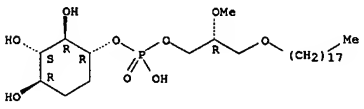
Absolute stereochemistry.

L31 ANSWER 23 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



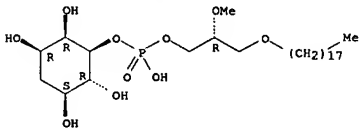
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-57-0 CAPLUS
CN D-epi-Inositol, 4-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

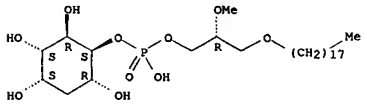
Absolute stereochemistry.



RN 701976-59-2 CAPLUS
CN D-allo-Inositol, 2-deoxy-, 6-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

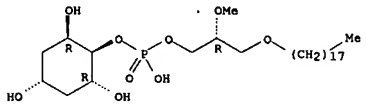
Absolute stereochemistry.

L31 ANSWER 23 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 701976-62-7 CAPLUS
CN Phosphoric acid, mono[2-methoxy-3-(octadecyloxy)propyl] mono[(1α,2R,4β,6R)-2,4,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

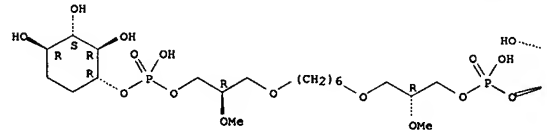
Absolute stereochemistry.



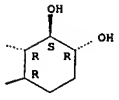
RN 701976-65-0 CAPLUS
CN Phosphoric acid, P,P'-[1,6-hexanediylbis[oxy[(2R)-2-methoxy-3,1-propanediyl]]] P,P'-bis[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

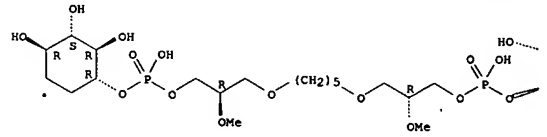


RN 701976-67-2 CAPLUS
CN Phosphoric acid, P,P'-[1,5-pentanediylbis[oxy[(2R)-2-methoxy-3,1-

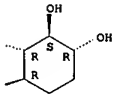
L31 ANSWER 23 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
propanediyl]]] P,P'-bis[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

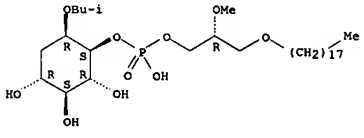


PAGE 1-B



RN 701976-68-3 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-(2-methylpropyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

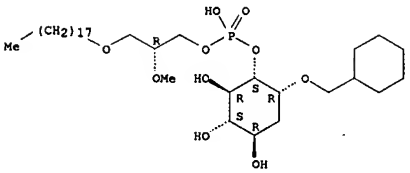
Absolute stereochemistry.



RN 701976-69-4 CAPLUS
CN L-chiro-Inositol, 1-O-(cyclohexylmethyl)-6-deoxy-, 2-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

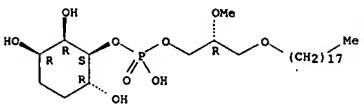
Absolute stereochemistry.

L31 ANSWER 23 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

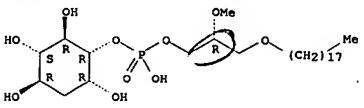
L31 ANSWER 24 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:1001605 CAPLUS
DOCUMENT NUMBER: 140:35923
TITLE: 3-Deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation thereof, and use for inhibition of cancer cell growth
INVENTOR(S): Kozikowski, Alan P.; Qiao, Lixin; Powis, Garth
PATENT ASSIGNEE(S): Arizona Board of Regents On Behalf of the University of Arizona, USA; Georgetown University School of Medicine
SOURCE: U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 339,948.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6667340 | B1 | 20031223 | US 2001-879765 | 20010612 |
| US 6245754 | B1 | 20010612 | US 1999-339948 | 19990625 |
| EP 1574216 | A1 | 20050914 | EP 2005-76269 | 19990625 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |
| US 2004192770 | A1 | 20040930 | US 2003-733115 | 20031211 |
| US 7153843 | B2 | 20061226 | | |
| PRIORITY APPLN. INFO.: | | | US 1998-90877P | P 19980626 |
| | | | US 1999-339948 | A2 19990625 |
| | | | US 2000-223421P | P 20000807 |
| | | | US 2000-223724P | P 20000808 |
| | | | US 2000-235269P | P 20000926 |
| | | | US 2000-235270P | P 20000926 |
| | | | EP 1999-927339 | A3 19990625 |
| | | | US 2001-879765 | A1 20010612 |

OTHER SOURCE(S): MARPAT 140:35923
AB The invention discloses the preparation and biol. activity of 3-deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth. The compds. of the invention are useful as antitumor agents.
IT 253440-95-8P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 253440-95-8 CAPLUS

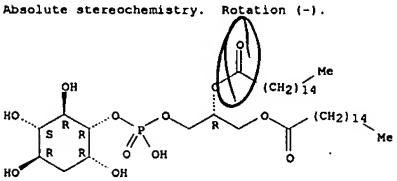
L31 ANSWER 24 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 162792-27-0
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

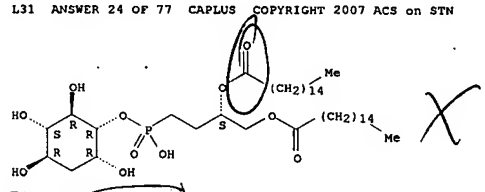
Absolute stereochemistry. Rotation (-).



IT 253440-94-7P 253440-97-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 253440-94-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3S)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate] (9CI) (CA INDEX NAME)

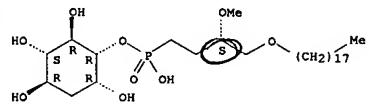
Absolute stereochemistry.

L31 ANSWER 24 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



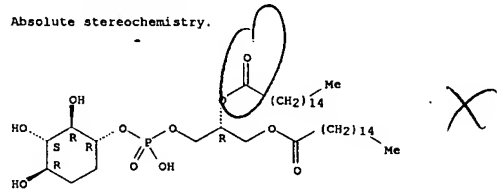
RN 253440-97-0 CAPLUS
CN Phosphonic acid, [(3S)-3-methoxy-4-(octadecyloxy)butyl]-, mono[(1R,2R,3S,4R,6R)-2,3,4,6-tetrahydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 197896-32-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 197896-32-5 CAPLUS
CN Hexadecanoic acid, (1R)-1-[[[hydroxy[[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl]oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester (9CI)
(CA INDEX NAME)

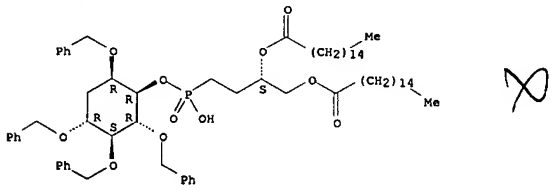
Absolute stereochemistry.



IT 253440-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl

L31 ANSWER 24 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
myo-inositol cycle, prepn., and use for inhibition of cancer cell growth)
RN 253440-93-6 CAPLUS
CN L-chiro-Inositol, 1-deoxy-2,3,4,6-tetrakis-O-(phenylmethyl)-, hydrogen [(3S)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

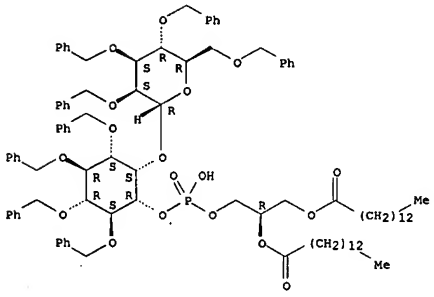
L31 ANSWER 25 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:963356 CAPLUS
DOCUMENT NUMBER: 140:164096
TITLE: Synthesis of phosphatidylinositol mannosides (PIMs)
AUTHOR(S): Stadelmaier, Andreas; Schmidt, Richard R.
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Konstanz, Konstanz, D-78457, Germany
SOURCE: Carbohydrate Research (2003), 338(23), 2557-2569
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:164096
AB Two strategies towards the synthesis of phosphatidylinositol mannosides (PIMs) were elaborated which permit selective access to the O-1-, O-2-, and the O-6 position of the myo-inositol residue. Starting materials are 1,2:5,6- and 1,2:4,5-di-O-cyclohexylidene-DL-myo-inositol, resp. In the latter case, the required assignment to the D- or L-series is based on the transformation of one enantiomer into known (-)-liriodentritol. The efficiency and potential versatility of the two approaches is exemplified in the synthesis of (D) PIMs and its (L)-pseudoenantiomer, both having myristoyl residues as part of the phosphatidyl moiety.
IT 652987-40-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of (D) and (L) phosphatidylinositol mannosides which are amendable to regioselective addns. on the O-6 position of the inositol moiety)
RN 652987-40-1 CAPLUS
CN D-myo-Inositol, 1,4,5,6-tetrakis-O-(phenylmethyl)-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, 3-[(2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate], compd. with N-methylmethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 579494-17-0
CMF C99 H129 O18 P

Absolute stereochemistry.

L31 ANSWER 25 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 124-40-3
CMF C2 H7 N

$H_3C-NH-CH_3$

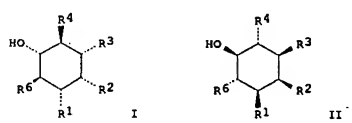
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L31 ANSWER 26 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:656778 CAPLUS
DOCUMENT NUMBER: 139:180298
TITLE: Preparation of substituted inositols and their use as phosphatidylinositol hexamannoside mimics and potential drug delivery agents
INVENTOR(S): Rademacher, Thomas William; Schmidt, Richard; Stadelmaier, Andreas
PATENT ASSIGNEE(S): Lascaux Pharmaceuticals Limited, UK
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003068789 | A1 | 20030821 | WO 2003-GB604 | 20030213 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003245767 | A1 | 20030904 | AU 2003-245767. | 20030213 |
| EP 1480991 | A1 | 20041201 | EP 2003-739562 | 20030213 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| US 2005143290 | A1 | 20050630 | US 2003-504605 | 20030213 |
| PRIORITY APPLN. INFO.: | | | GB 2002-3535 A | 20020214 |
| | | | WO 2003-GB604 W | 20030213 |

OTHER SOURCE(S): MARPAT 139:180298
GI



AB Inositol phosphate esters and conjugates I and II, wherein R1 is hydroxyl, phosphate, phosphatidic acid or a phosphate ester; R2 is a sugar moiety; R3 is are selected from hydroxyl or phosphate; R4 and/or R6 is or are independently selected from: an amino acid; or a peptide or polypeptide; or a group having the general formula: O-(CH2)n-CH(NR7R8)-CO2X, wherein:
n

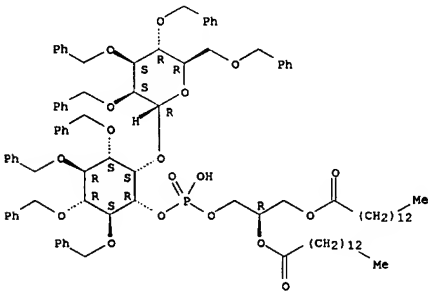
L31 ANSWER 26 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
is an integer between 1 and 10, R7 and R8 are independently selected from hydrogen, nitrogen, acyl or alkyl; and X is hydrogen, alkyl or a cation where the terminal group is CO2-; or a substituted or unsubstituted arom. group, formed between the compds. and a coupling partner are disclosed, in particular compds. based on a myo-inositol which is substituted at position 1 with a phosphate ester group, at position 2 with a sugar group and at position 4 and/or position 6 with an amino acid group. The compds. are based on the structure of phosphatidylinositol hexamannosides (PIM6) of Mycobacteria and may be used as mimics of the naturally occurring PIMs in order to induce biol. responses normally attributed to the natural compd. or may be used as biol. inert carriers in order to deliver specific pharmaceutically active compds. to lipid rafts/caveolae (no data). Thus, triethylammonium-[2-O-(α-D-mannopyranosyl)-L-myo-inosit-1-yl]-[(2R)-2,3-bis(myristoyloxy)propyl]-phosphate was prepd. as phosphatidylinositol hexamannoside mimic and potential drug delivery agent.

IT 579494-17-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted inositols and their use as phosphatidylinositol hexamannoside mimics and potential drug delivery agents)

RN 579494-17-0 CAPLUS

CN D-myo-Inositol, 1,4,5,6-tetrakis-O-(phenylmethyl)-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, 3-[(2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

L31 ANSWER 26 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 27 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:388780 CAPLUS
DOCUMENT NUMBER: 139:270468
TITLE: Specific inhibition of the Akt1 pleckstrin homology domain by D-3-deoxy-phosphatidyl-myo-inositol analogues
AUTHOR(S): Meuillet, Emmanuelle J.; Mahadevan, Daruka; Vankayalapati, Hariprasad; Berggren, Margareta; Williams, Ryan; Coon, Amy; Kozikowski, Alan P.; Powis, Garth
CORPORATE SOURCE: Arizona Cancer Center, University of Arizona, Tucson, AZ, 85724, USA
SOURCE: Molecular Cancer Therapeutics (2003), 2(4), 389-399
CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Activation of Akt (protein kinase B), a Ser/Thr protein kinase that promotes cell survival, has been linked to tumorigenesis. Akt is activated by phosphorylation after binding of its pleckstrin homol. (PH) domain to plasma membrane phosphatidyl-myo-inositol-3-phosphates, formed by phosphoinositide-3-kinase. We report a novel strategy to inhibit Akt activation based on the use of D-3-deoxy-phosphatidyl-myo-inositols (DPIs) that cannot be phosphorylated on the 3-position of the myo-inositol ring. We have studied the DPIs, DPI 1-[(R)-2,3-bis(hexadecanoyloxy)propyl hydrogen phosphate], its ether lipid derivative DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl hydrogen phosphate] (DPIEL), and its carbonate derivative DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl carbonate]. We demonstrate in platelet-derived growth factor-stimulated mouse NIH3T3 cells that the DPIs bind to the PH domain of Akt, trapping it in the cytoplasm and thus preventing Akt activation. DPIEL did not inhibit myristylated-Akt, a constitutively active membrane-bound Akt expressed in NIH3T3 cells, and cell growth was not inhibited, unlike in wild-type NIH3T3 cells. Mol. modeling and docking studies show that DPIEL binds with much higher affinity to Akt's PH domain as compared with DPI and DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl carbonate]. This study shows that the DPIs are a novel class of growth inhibitory agents with a novel mechanism of action through binding to the PH domain of Akt and inhibition of Akt activation.

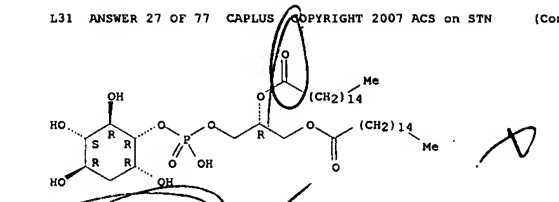
IT 162792-27-0 253440-95-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of Akt1 pleckstrin homol. domain by deoxyphosphatidyl-myo-inositol analogs)

RN 162792-27-0 CAPLUS

CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

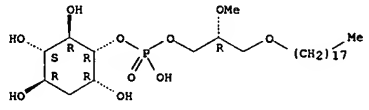
L31 ANSWER 27 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 253440-95-8 CAPLUS

CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 28 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:862524 CAPLUS
DOCUMENT NUMBER: 138:267584
TITLE: Further probing of the substrate specificities and inhibition of enzymes involved at an early stage of glycosylphosphatidylinositol (GPI) biosynthesis
AUTHOR(S): Crossman, Arthur; Paterson, Michael J.; Ferguson, Michael A. J.; Smith, Terry K.; Brimacombe, John S.
CORPORATE SOURCE: School of Life Sciences (Chemistry), University of Dundee, Dundee, DD1 4HN, UK
SOURCE: Carbohydrate Research (2002), 337(21-23), 2049-2059
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:267584

AB 1-D-6-O-(2-Amino-2-deoxy-α-D-glucopyranosyl)-1-O-hexadecyl-myo-inositol (14), 1-d-6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-(octadecyl phosphate) (18), 1-D-6-O-(2-amino-2-deoxy-β-D-glucopyranosyl)-myo-inositol 1-(1,2-di-O-hexadecanoyl-sn-glycerol 3-phosphate) (24), 1-D-6-O-(2-amino-2-deoxy-α-D-mannopyranosyl)-myo-inositol 1-(1,2-di-O-hexadecanoyl-sn-glycerol 3-phosphate) (30) and the corresponding 2-amino-2-deoxy-α-D-galactopyranosyl analog 36 have been prepared and tested in cell-free assays as substrate analogs/inhibitors of α-(1 4)-D-mannosyltransferases that are active early on in the glycosylphosphatidylinositol (GPI) biosynthetic pathways of Trypanosoma brucei and HeLa (human) cells. The corresponding N-acetyl derivs. of these compds. were similarly tested as candidate substrate analogs/inhibitors of the N-deacetylases present in both systems. Following on from an early study, 1-L-6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-2-O-methyl-myo-inositol 1-(1,2-di-O-hexadecanoyl-sn-glycerol 3-phosphate) (44) was prepared and tested as an inhibitor of the trypanosomal α-(1 4)-D-mannosyltransferase. A brief summary of the biol. evaluation of the various analogs is provided.

IT 503177-41-1P 503177-45-5P 503177-48-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(substrate specificities and inhibition of α-(1 4)-D-mannosyltransferase and N-deacetylase enzymes involved at early stage of glycosylphosphatidylinositol biosynthesis in human and Trypanosoma brucei)

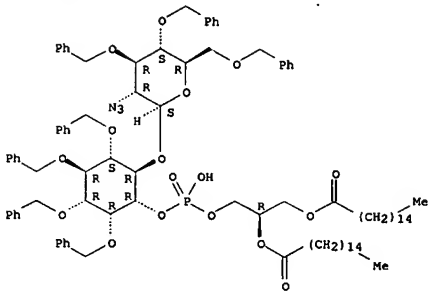
RN 503177-41-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-β-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 503177-40-0
CMF C96 H130 N3 O17 P

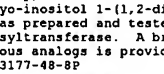
Absolute stereochemistry. Rotation (-).

L31 ANSWER 28 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N



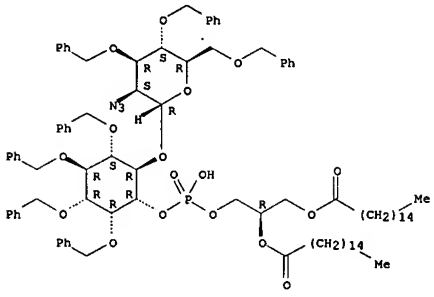
RN 503177-45-5 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-mannopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 503177-44-4
CMF C96 H130 N3 O17 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 28 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N



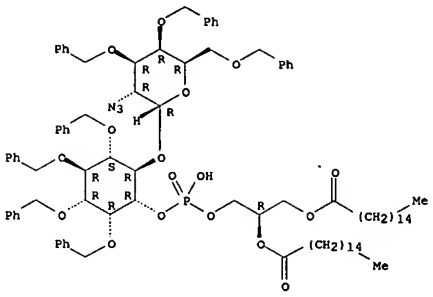
RN 503177-48-8 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-galactopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 503177-47-7
CMF C96 H130 N3 O17 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 28 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

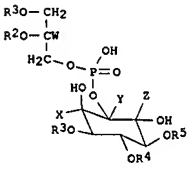


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 29 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:312045 CAPLUS
DOCUMENT NUMBER: 136:325777
TITLE: Preparation of labeled phosphoinositides and analogs
INVENTOR(S): Aneja, Rajindra
PATENT ASSIGNEE(S): Nutrimed Biotech, USA
SOURCE: U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6376697 | B1 | 20020423 | US 1999-292242 | 19990415 |
| US 7037486 | B1 | 20060502 | US 2002-56188 | 20020124 |
| PRIORITY APPLN. INFO.: | | | US 1998-81847P P | 19980415 |
| | | | US 1999-292242 A3 | 19990415 |

OTHER SOURCE(S): MARPAT 136:325777
GI

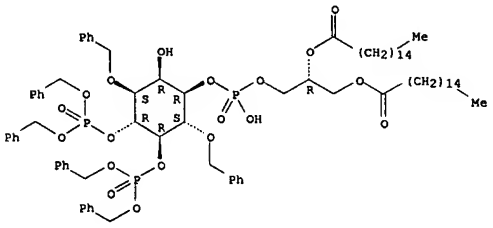


I

AB The present invention provides novel deuterium, phosphorus, or sulfur-labeled phosphoinositides I were prepared wherein R1 and R2 are fatty acid, alkyl, H; R3-R5 are independently H, Q(T)(OH)2; Q is P, 32P, 33P; T is O, 35S; W, X, Y, Z are independently H, 2H, 3H, comprising cellular phosphoinositides and analogs tagged with stable or radioactive isotopes. The present invention also provides novel methods for the preparation of the said phosphoinositides by syntheses, and novel key intermediates of synthesis; the novel methods of synthesis are applied also for the preparation of the phosphoinositides in non-labeled form. In addition, the present invention discloses a class of novel compds. as isotope labeled key precursors of labeled phosphoinositides. These precursors are derivs. of the target phosphoinositides, labeled with stable or radioactive isotopes,

L31 ANSWER 29 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
wherein OH and phosphate groups are blocked with temporary protecting groups. Thus, 1D-2-(1',2'-O-dipalmitoyl-sn-glycero-3'-phospho)-3,6-di-O-benzyl-1-myo-inosose-4,5-bis(dibenzyl phosphate) was prepd.
IT 411225-06-4P 411225-10-0P 411225-11-1P
411225-12-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of labeled phosphoinositides and analogs)
RN 411225-06-4 CAPLUS
CN D-myo-Inositol, 3,6-bis(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

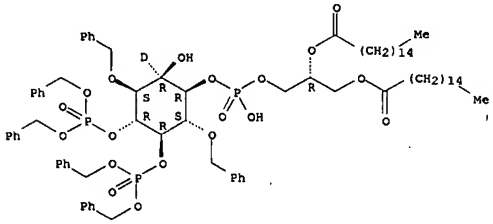
Absolute stereochemistry.



RN 411225-10-0 CAPLUS
CN D-myo-Inositol-2-C-d, 3,6-bis(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

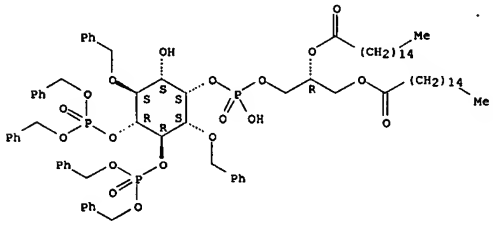
Absolute stereochemistry.

L31 ANSWER 29 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 411225-11-1 CAPLUS
CN D-myo-Inositol, 3,6-bis(phenylmethyl)-, 2-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

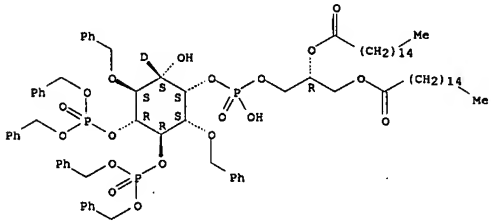
Absolute stereochemistry.



RN 411225-12-2 CAPLUS
CN D-myo-Inositol-1-C-d, 3,6-bis(phenylmethyl)-, 2-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 29 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

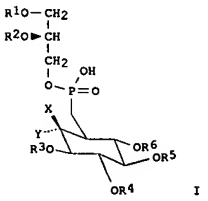


REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 30 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:355095 CAPLUS
DOCUMENT NUMBER: 134:340656
TITLE: Preparation of glycerophosphatidylinositols as molecular probes and modulators for phosphatidylinositol-specific phospholipase C (PI-PLC) and phosphatidylinositol 3-kinase (PI 3-kinase)
INVENTOR(S): Aneja, Rajindra
PATENT ASSIGNEE(S): Nutrimed Biotech, USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6232486 | B1 | 20010515 | US 1997-872222 | 19970610 |
| US 6384260 | B1 | 20020507 | US 2001-826396 | 20010403 |
| PRIORITY APPLN. INFO.: | | | US 1996-19651P P | 19960611 |
| | | | US 1997-872222 A1 | 19970610 |

OTHER SOURCE(S): MARPAT 134:340656
GI



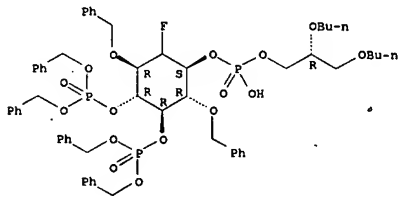
I

AB This invention provides analogs of phosphatidylinositol-phosphates I wherein at least one of R3, R4, R5, R6 is P(O)(OH)2, and wherein (a) X = F, Cl, Br, OC(O)R, OR, or OP(O)(OH)2, and Y = H; or X = Y = H; or (b) X = H, and Y = F, Cl, Br, OC(O)R, OR, or OP(O)(OH)2 ; or (c) X = Y = F or O; where R = alkyl, [especially Me or Et] alkenyl, alkynyl, ω-aminoalkyl, N-substituted-ω-aminoalkyl or N,N-disubstituted-ω-aminoalkyl; and wherein (d) R1 = RC(O) or R, R2 = R'C(O) or R' where R, R' = alkyl or alkenyl; and wherein (e) R3 = H, or P(O)(OH)2 (f) R4 = H, or P(O)(OH)2 (g) R5 = H, or P(O)(OH)2 (h) R6 = H, P(O)(OH)2, ω-aminoalkyl, ω-aminoalkenyt, ω.-sulthydrylalkyl, ω-carboxyalkyl, ω.-(4-azidosalicyl amido)-alkyl, alkyl-aminotluorophor, alkyl-amidofluorophor, or alkyl-fluorophor, modified at one or more selected inositol-hydroxyls and optionally carrying reporter or anchoring groups attached in the lipid or the inositol residues, and, the synthetic intermediates and methods for the prepn. of these analogs. The analogs are useful as research reagents in biomedical studies related to structure, function and therapeuticals, including ref. materials for analyzing the metabolic products and efficacy studies of 2- and/or 3-hydroxyl modified inositols and phosphatidylinositols as drug candidates. Thus, 1D-2-deoxy-fluoro-1-O-(1',2'-di-O-palmitoyl-sn-glycero-3'-O-phospho)-myo/scyllo-inositol 4,5-bis-O-phosphate was prepd. as modulators for phosphatidylinositol-specific phospholipase C and phosphatidylinositol 3-kinase (no data).

IT 337955-75-6P 337955-79-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of glycerophosphatidylinositols as mol. probes and modulators for phosphatidylinositol-specific phospholipase C and phosphatidylinositol 3-kinase)

RN 337955-75-6 CAPLUS
CN D-myo-Inositol, 2-deoxy-2-fluoro-3,6-bis-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 1-[(2R)-2,3-dibutoxypropyl hydrogen phosphate], (2ξ)- (9CI) (CA INDEX NAME)

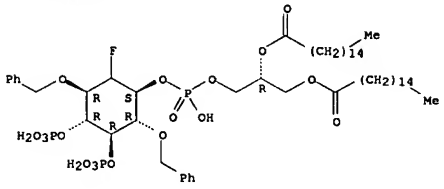
Absolute stereochemistry.



RN 337955-79-0 CAPLUS
CN D-myo-Inositol, 2-deoxy-2-fluoro-3,6-bis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate), (2ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

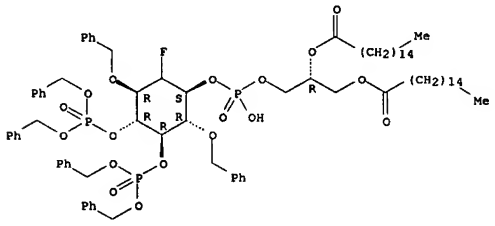
L31 ANSWER 30 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 337955-77-8P 337955-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of glycerophosphatidylinositols as mol. probes and modulators for phosphatidylinositol-specific phospholipase C and phosphatidylinositol 3-kinase)

RN 337955-77-8 CAPLUS
CN D-myo-Inositol, 2-deoxy-2-fluoro-3,6-bis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate], (2ξ)- (9CI) (CA INDEX NAME)

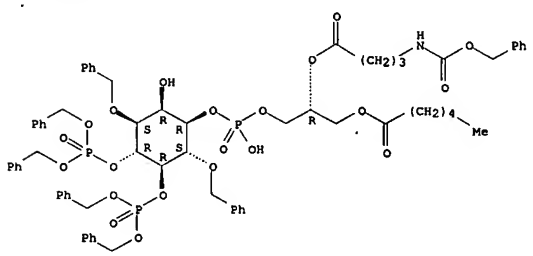
Absolute stereochemistry.



RN 337955-89-2 CAPLUS
CN D-myo-Inositol, 3,6-bis-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 1-[(2R)-3-[(1-oxohexyl)oxy]-2-[1-oxo-4-[[(phenylmethoxy)carbonyl]amino]butoxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 30 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

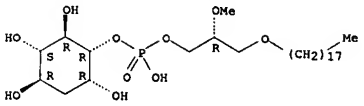


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 31 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:242518 CAPLUS
DOCUMENT NUMBER: 135:101840
TITLE: High-performance liquid chromatographic analysis for a non-chromophore containing phosphatidyl inositol analog, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, using indirect UV detection
AUTHOR(S): He, J.; Cheung, A. P.; Wang, E.; Fang, K.; Liu, P.
CORPORATE SOURCE: SRI International, Menlo Park, CA, 94025-3493, USA
SOURCE: Journal of Chromatography, A (2001), 913(1-2), 355-363
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phosphatidylinositide-3-kinase (PI3 kinase) is an important constituent of growth factor regulation. It is also involved in oncogene signaling pathways. An ether-containing phosphatidyl inositol(PI) analog, OMDPI, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, is a potent inhibitor of this pathway and may be clin. useful in the treatment of a variety of neoplasms. OMDPI is currently being studied as an antitumor agent by the National Cancer Institute, NIH. OMDPI, a nonchromophore-containing PI analog, is not directly adaptable to the commonly used UV detection of HPLC. This paper reports the development and validation of an HPLC assay for OMDPI based on indirect UV detection, in which a UV-absorbing ion-pair reagent (the probe), protriptyline, is added to the mobile phase to induce a signal for the compound The method is sensitive (limit of detection <5 μL of 1 μg/mL or 5 ng), precise (relative standard deviation <2.5%), linear (r2 = 0.9995) and accurate (error<0.7%). It is superior to refractive index detection and evaporative light scattering detection in either sensitivity or linearity and does not require special equipment.
IT 253440-95-8, 1-[(1-O-Octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol
RL: ANT (Analyte); ANST (Analytical study)
(high-performance liquid chromatog. anal. for a non-chromophore-containing phosphatidyl inositol analog, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, using indirect UV detection)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

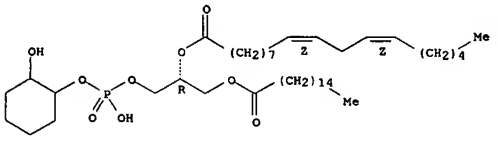
L31 ANSWER 31 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 32 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:93086 CAPLUS
DOCUMENT NUMBER: 134:322504
TITLE: The substrate requirements of phospholipase D
AUTHOR(S): Bossi, L.; D'Arrigo, P.; Pedrocchi-Fantoni, G.; Mele, A.; Servi, S.; Leiros, I.
CORPORATE SOURCE: Centro di Studio sulle Sostanze Organiche Naturali, Dipartimento di Chimica, CNR, Politecnico di Milano, Milan, 20131, Italy
SOURCE: Journal of Molecular Catalysis B: Enzymatic (2001), 11(4-6), 433-438
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The hydrolysis rates of different diphosphates, compared with the one observed with natural phosphatidylcholine, are used to identify the mol. basis for phospholipase D (PLD) catalysis. Exptl. data strongly support the idea that PLD is a rather generic phosphodiesterase with very wide substrate specificity and a net preference for lipophilic substrates. The presence of choline in the polar head is not required for activity although it improves hydrolysis efficiency. Choline esters are found to be substrates for PLD hydrolysis, but only with long chain fatty acids.
IT 336786-72-2P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(structure-activity relationships of phospholipase D substrates)
RN 336786-72-2 CAPLUS
CN 9,12-Octadecadienoic acid (9Z,12Z)-, (1R)-1-[[[hydroxy[(2-hydroxycyclohexyl)oxy]phosphinyl]oxy]methyl]-2-[(1-oxohexadecyl)oxy]ethyl ester (9CI) (CA INDEX NAME)

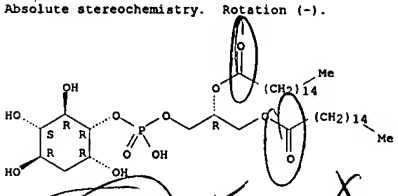
Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 33 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:83663 CAPLUS
DOCUMENT NUMBER: 134:252547
TITLE: 3-Deoxy-3-substituted-D-myo-inositol imidazolyl ether lipid phosphates and carbonate as inhibitors of the phosphatidylinositol 3-kinase pathway and cancer cell growth
AUTHOR(S): Hu, Y.; Meuillet, E. J.; Berggren, M.; Powis, G.; Kozikowski, A. P.
CORPORATE SOURCE: Drug Discovery Program, Department of Neurology, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(2), 173-176
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:252547
AB 3-Modified D-myo-inositol imidazolyl ether lipid phosphates and a carbonate were synthesized and evaluated as inhibitors of PI3-K and Akt. These data are presented along with IC50 values for the inhibition of the growth of three cancer cell lines. 3-Modified D-myo-inositol imidazolyl ether lipid phosphates and a carbonate were synthesized and evaluated as inhibitors of PI3-K, Akt, and cancer cell growth.
IT 162792-27-0 253440-95-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 3-deoxy-3-substituted-D-myo-inositol imidazolyl ether lipid phosphates and carbonate as inhibitors of the phosphatidylinositol 3-kinase pathway and cancer cell growth)
RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

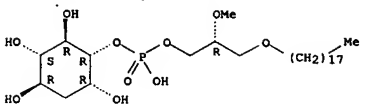
Absolute stereochemistry. Rotation (-).



RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

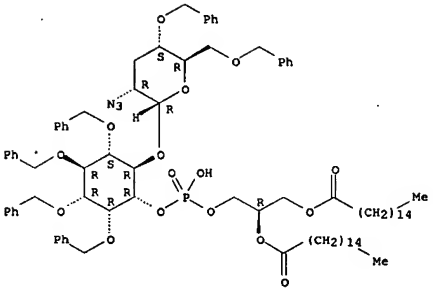
Absolute stereochemistry.

L31 ANSWER 33 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 34 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 34 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:895665 CAPLUS
DOCUMENT NUMBER: 134:163245
TITLE: Synthesis of 3'-, 4'- and 6'-deoxy and other analogues
of D-glucosaminylphosphatidylinositol
AUTHOR(S): Borissow, C. N.; Smith, T. K.; Ferguson, M. A. J.; Brimacombe, J. S.
CORPORATE SOURCE: Department of Chemistry, University of Dundee, Dundee,
DD1 4HN, UK
SOURCE: Tetrahedron Letters (2001), 42(1), 121-123
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:163245
AB Deoxy and other analogs of D-glucosaminylphosphatidylinositol have been synthesized and tested as substrates or inhibitors of a de-N-acetylase and
mannosyltransferase (MT-1) involved in the biosynthesis of the glycosylphosphatidylinositol (GPI) membrane anchor of the parasite Trypanosoma brucei.
IT 324739-91-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of deoxy and other analogs of D-glucosaminylphosphatidylinositol as substrates or inhibitors of de-N-acetylase and mannosyltransferase)
RN 324739-91-5 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2,3-dideoxy-4,6-bis-O-(phenylmethyl)-α-D-ribo-hexopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-{(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate}, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

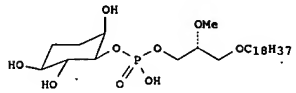
CM 1

CRN 324739-90-4
CMF C89 H124 N3 O16 P

Absolute stereochemistry. Rotation (+).

Hu.

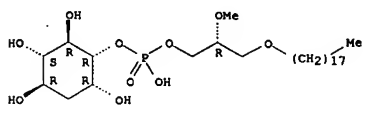
L31 ANSWER 35 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:498487 CAPLUS
DOCUMENT NUMBER: 134:42338
TITLE: Synthesis and Akt kinase inhibitory properties of a ld-3,4-dideoxyphosphatidylinositol ether lipid
AUTHOR(S): Hu, Y.; Meuillet, E. J.; Qiao, L.; Berggren, M. M.; Powis, G.; Kozikowski, A. P.
CORPORATE SOURCE: Department of Neurology, Drug Discovery Program, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Tetrahedron Letters (2000), 41(39), 7415-7418
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:42338
GI



I

AB 1D-3,4-Dideoxyphosphatidylinositol ether lipid I (X = H) (DDPIEL), a PI analog, was synthesized through a sequence of protection/deprotection protocols and two Barton deoxygenation reactions, starting from L-(-)-quebrachitol. DDPIEL I is 18-fold more potent than its monodeoxy counterpart I (X = OH) (DPIEL) in the inhibition of PI3-K.
IT 253440-95-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); BIOL (Biological study)
(synthesis and Akt kinase inhibitory properties of a ld-3,4-dideoxyphosphatidylinositol ether lipid)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

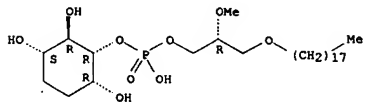
Absolute stereochemistry.



IT 310872-32-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and Akt kinase inhibitory properties of a

L31 ANSWER 35 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1d-3,4-dideoxyphosphatidylinositol ether lipid)
RN 310872-32-3 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



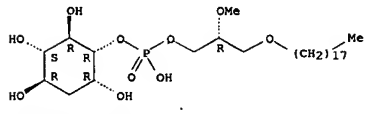
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 36 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:481805 CAPLUS
DOCUMENT NUMBER: 133:217271
TITLE: 3-(Hydroxymethyl)-Bearing Phosphatidylinositol Ether Lipid Analogues and Carbonate Surrogates Block PI3-K, Akt, and Cancer Cell Growth
AUTHOR(S): Hu, Yaohong; Qiao, Lixin; Wang, Shaomeng; Rong, Su-bao; Meuillet, Emmanuelle J.; Berggren, Margareta; Gallegos, Alfred; Powis, Garth; Kozikowski, Alan P.
CORPORATE SOURCE: Drug Discovery Program Department of Neurology, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(16), 3045-3051
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phosphatidylinositol 3-kinase (PI3-K) phosphorylates the 3-position of phosphatidylinositol to give rise to three signaling phospholipids. Binding of the pleckstrin homol. (PH) domain of Akt to membrane PI(3)P's causes the translocation of Akt to the plasma membrane bringing it into contact with membrane-bound Akt kinase (PDK1 and 2), which phosphorylates and activates Akt. Akt inhibits apoptosis by phosphorylating Bad, thus promoting its binding to and blockade of the activity of the cell survival factor Bcl-x. Herein we present the synthesis and biol. activity of several novel phosphatidylinositol analogs and demonstrate the ability of the carbonate group to function as a surrogate for the phosphate moiety. Due to a combination of their PI3-K and Akt inhibitory activities, the PI analogs proved to be good inhibitors of the growth of various cancer cell lines with IC50 values in the 1-10 μM range. The enhanced Akt inhibitory activity of the axial hydroxymethyl-bearing analog compared to its equatorial counterpart is rationalized based upon postulated differences in the H-bonding patterns of these compds. in complex with a homol. modeling generated structure of the PH domain of Akt. This work represents the first attempt to examine the effects of 3-modified PI analogs on these two crucial cell signaling proteins, PI3-K and Akt, in an effort to better understand their cell growth inhibitory properties.
IT 253440-95-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and structure activity relations of phosphatidylinositol ether lipid analogs and carbonate surrogates that block PI3-K, Akt kinase, and cancer cell growth)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Hu - previous O.A

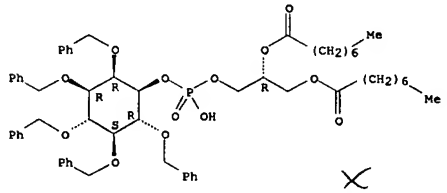
L31 ANSWER 36 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 37 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:128353 CAPLUS
DOCUMENT NUMBER: 132:293946
TITLE: Practical unequivocal synthesis of phosphatidyl-myo-inositols
AUTHOR(S): Aneja, Rajindra; Aneja, Sarla G.
CORPORATE SOURCE: Functional Lipids Division, Nutrimed Biotech, Langmuir Laboratory, Cornell University Research Park, Ithaca, NY, 14850-1257, USA
SOURCE: Tetrahedron Letters (2000), 41(6), 847-850
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The direct phosphatidylation of 1D-2,3,4,5,6-penta-O-benzyl-myo-inositol with sn-3-phosphatidic acid and subsequent hydrogenolytic debenzylation produces 1D-1-(sn-3-phosphatidyl)-myo-inositol in excellent yield (>90%) and unequivocal structural and stereochem. purity, and, is readily adaptable for large scale production
IT 264125-32-8P 264125-33-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical unequivocal synthesis of phosphatidyl-myo-inositols)
RN 264125-32-8 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxooctyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

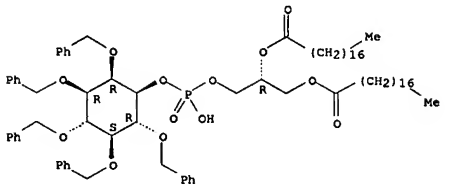
Absolute stereochemistry. Rotation (+).



RN 264125-33-9 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 37 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



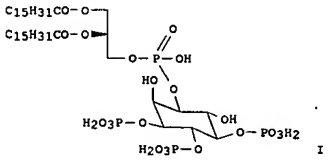
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 38 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:83121 CAPLUS
DOCUMENT NUMBER: 132:108223
TITLE: Synthesis of D-3-phosphorylated phosphoinositides and analogs
INVENTOR(S): Aneja, Rajindra
PATENT ASSIGNEE(S): Nutrimed Biotech, USA
SOURCE: U.S., 20 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

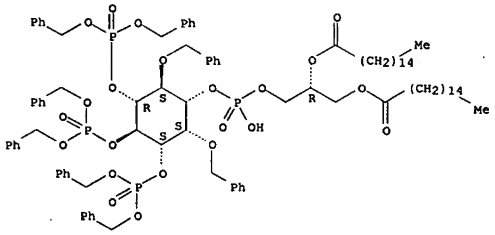
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6020506 | A | 20000201 | US 1997-862865 | 19970523 |
| US 6096916 | A | 20000801 | US 1999-361874 | 19990727 |
| US 38334 | E1 | 20031125 | US 2002-62984 | 20020131 |
| PRIORITY APPLN. INFO.: | | | US 1996-18319P P | 19960524 |
| | | | US 1997-862865 A3 | 19970523 |

OTHER SOURCE(S): MARPAT 132:108223
GI



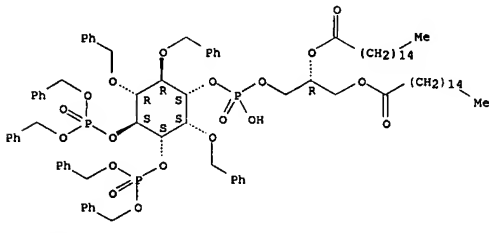
AB Disclosed are unique starting materials, reaction sequences and intermediate compds. for the preparation of D-3-phosphorylated phosphoinositides (3-PPI) of unambiguous structure and absolute stereochem.
Thus, phosphoinositide I was prepared for the development of diagnostics and
therapeutics based on the roles of 3-PPI in intracellular signaling (no data).
IT 188112-77-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of phosphorylated phosphoinositides and analogs)
RN 188112-77-8 CAPLUS
CN D-myo-Inositol, 2,6-bis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3,4,5-tris[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 196304-59-3P 255384-14-6P 255384-15-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of phosphorylated phosphoinositides and analogs)
RN 196304-59-3 CAPLUS
CN D-myo-Inositol, 2,5,6-tris-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3,4-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

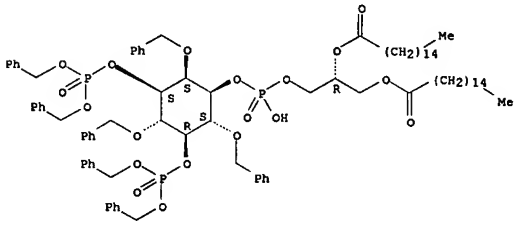
Absolute stereochemistry. Rotation (+).



RN 255384-14-6 CAPLUS
CN D-myo-Inositol, 2,4,6-tris-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

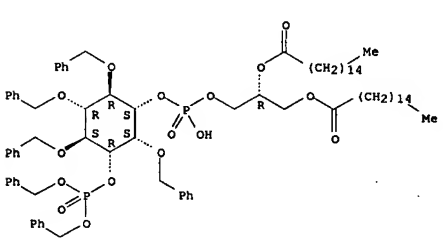
Absolute stereochemistry.

L31 ANSWER 38 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 255384-15-7 CAPLUS
CN D-myo-Inositol, 2,4,5,6-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3-[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 39 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:15026 CAPLUS
DOCUMENT NUMBER: 132:59159
TITLE: Inhibitors of phosphatidyl-myo-insitol cycle for cancer treatment
INVENTOR(S): Kozikowski, Alan P.; Qioa, Lixin; Powis, Garth
PATENT ASSIGNEE(S): Georgetown University, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000000206 | A1 | 20000106 | WO 1999-US12824 | 19990625 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 9944271 | A | 20000117 | AU 1999-44271 | 19990607 |
| CA 2335995 | A1 | 20000106 | CA 1999-2335995 | 19990625 |
| EP 1119364 | A1 | 20010801 | EP 1999-927339 | 19990625 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| EP 1574216 | A1 | 20050914 | EP 2005-76269 | 19990625 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |

PRIORITY APPLN. INFO.: US 1998-90877P P 19980626
EP 1999-927339 A3 19990625
WO 1999-US12824 W 19990625

OTHER SOURCE(S): MARPAT 132:59159

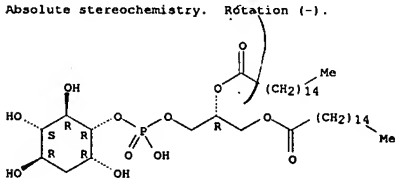
AB The present invention relates to the preparation and biol. activity of 3-deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth. The compds. of the present invention are useful as anti-tumor agents which effectively inhibit the growth of mammalian cells. For example, 1-O-octadecyl-2-O-methyl-sn-glycero-3-phospho-myo-inositol (OMDPI) administered by a 4 or 5 day daily i.p. schedule resulted in a 60% inhibition of the growth of human MCF-7 breast cancer and a 67% inhibition of the growth of HT-29 colon tumor xenografts implanted in SCID mice. The activity of OMDPI administered by a 10 day schedule provided 80% inhibition of the growth of MCF-7 xenografts.

IT 253440-94-7P 253440-95-8P 253440-97-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L31 ANSWER 39 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors of phosphatidylinositol signaling for cancer treatment)

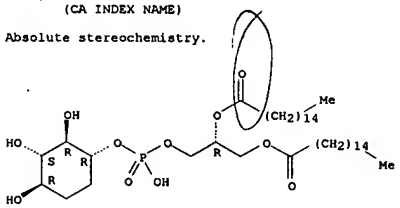
RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 197896-32-5 CAPLUS
CN Hexadecanoic acid, (1R)-1-[[[hydroxy[[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl]oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 253440-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(inhibitors of phosphatidylinositol signaling for cancer treatment)

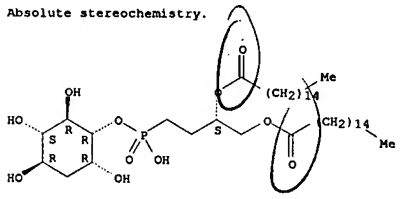
RN 253440-93-6 CAPLUS
CN L-chiro-Inositol, 1-deoxy-2,3,4,6-tetrakis-O-(phenylmethyl)-, hydrogen [(3S)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 39 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibitors of phosphatidylinositol signaling for cancer treatment)

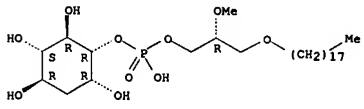
RN 253440-94-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3S)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

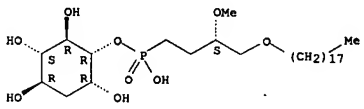
Absolute stereochemistry.



SAMPLE
2 cmpds

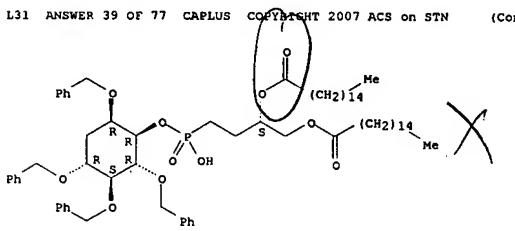
RN 253440-97-0 CAPLUS
CN Phosphonic acid, [(3S)-3-methoxy-4-(octadecyloxy)butyl]-, mono[(1R,2R,3S,4R,6R)-2,3,4,6-tetrahydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 162792-27-0 197896-32-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L31 ANSWER 39 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 40 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:804893 CAPLUS
DOCUMENT NUMBER: 132:152056
TITLE: Parasite glycoconjugates, Part 10. Synthesis of some second-generation substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors
AUTHOR(S): Crossman, Arthur, Jr.; Brimacombe, John S.; Ferguson, Michael A. J.; Smith, Terry K.
CORPORATE SOURCE: Department of Chemistry, University of Dundee, Dundee, DD1 4HN, UK
SOURCE: Carbohydrate Research (1999), 321(1-2), 42-51
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1-D-6-O-(2-Amino-2-deoxy-α-D-glucopyranosyl)-2-O-octyl-myo-inositol 1-(1,2-di-O-hexadecanoyl-sn-glycerol 3-phosphate) (I) and the corresponding 2-O-hexadecyl-D-myo-inositol (II) have been prepared as substrate analogs of an early intermediate in the biosynthetic pathway of glycosylphosphatidylinositol (GPI) membrane anchors. 1-D-6-O-(2-Amino-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-(1,2-di-O-octyl-sn-glycerol 3-phosphate) has also been prepared as a substrate analog. Biol. evaluation of the analogs I and II revealed that they are neither substrates nor inhibitors of GPI biosynthetic enzymes in the human (HeLa) cell-free system but are potent inhibitors at different stages of GPI biosynthesis in the Trypanosoma brucei cell-free system.

IT 256922-39-1P 257602-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of some second-generation substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors)

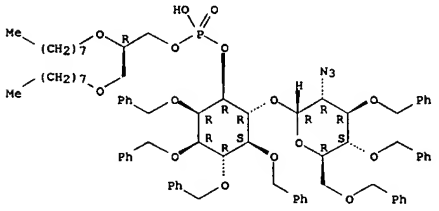
RN 256922-39-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis(octyloxy)propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 256922-38-0
CMF C80 H102 N3 O15 P

Absolute stereochemistry. Rotation (+).

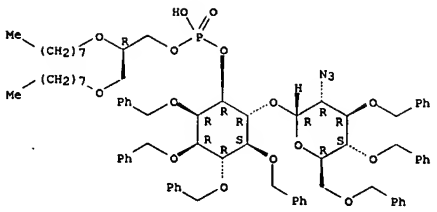
L31 ANSWER 40 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 40 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

RN 257602-83-8 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis(octyloxy)propyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

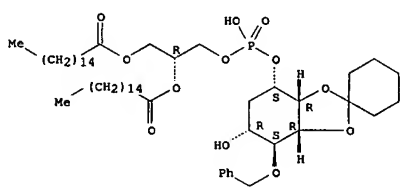
L31 ANSWER 41 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:688003 CAPLUS
DOCUMENT NUMBER: 132:50186
TITLE: Synthesis of deoxy phosphatidylinositol analogs and phosphonate isosters of ins(1,4,5)P3
AUTHOR(S): De Almeida, Mauro Vieira; Cleophax, Jeannine; Gateau-Olesker, Alice; Prestat, Guillaume; Dubreuil, Didier; Gero, Stephane D.
CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, C.N.R.S., Gif-sur-Yvette, 91198, Fr.
SOURCE: Tetrahedron (1999), 55(45), 12997-13010
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of phosphatidylinositol analogs, 6-deoxy Ins 1-(1,2-di-O-palmitoyl-sn-glycero)phosphate and 4,5-bisphosphate derivs. is presented. Two series of phosphonate isosters, 6-deoxy Ins(1)-butylphosphonate and 6-deoxy Ins(1)-C-methylenephosphonate as well as its 4,5-bisphosphate analog were also prepared All phosphoinositide analogs were obtained from cyclohexanone polyol derived from the D-galactose. Modification of charge distribution at position 1 of PtdIns and InsP derivs., by replacement of a P-OH group by an alkyl substitution or a P-C bond, resistant to cleavage by lipases, could induce inhibition of activity at further strategic enzymic levels of the inositide cascade.

IT 252868-88-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deoxy phosphatidylinositol analogs and phosphonate isosters of D-myo-inositol-1,4,5-trisphosphate)

RN 252868-88-5 CAPLUS
CN D-epi-Inositol, 4,5-O-cyclohexylidene-2-deoxy-6-O-(phenylmethyl)-, 3-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

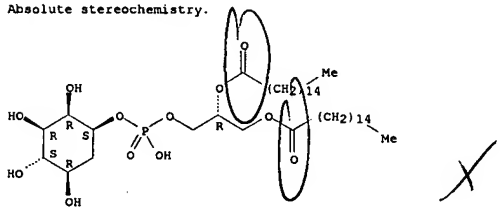


IT 252877-09-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deoxy phosphatidylinositol analogs and phosphonate isosters of D-myo-inositol-1,4,5-trisphosphate).

RN 252877-09-1 CAPLUS

L31 ANSWER 41 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN D-epi-Inositol, 2-deoxy-, 3-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 42 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:64950 CAPLUS
DOCUMENT NUMBER: 130:135002
TITLE: Dual specificity phosphatase PTEN and methods of use and structure of PTEN gene
INVENTOR(S): Tonks, Nicholas K.; Myers, Michael P.
PATENT ASSIGNEE(S): Cold Spring Harbor Laboratory, USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9902704 | A2 | 19990121 | WO 1998-US14205 | 19980708 |
| WO 9902704 | A3 | 19990401 | | |

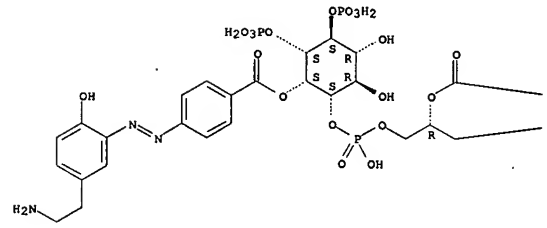
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| AU 9884794 | A | 19990208 | AU 1998-84794 | 19980708 |
| PRIORITY APPLN. INFO.: | | | US 1997-51908P | P 19970708 |
| | | | US 1998-90984P | P 19980629 |
| | | | WO 1998-US14205 | W 19980708 |

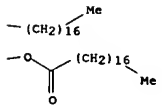
AB PTEN proteins and altered PTEN proteins, and the nucleic acid mols. encoding them are described. PTEN is a protein phosphatase and is a tumor suppressor with sequence homol. to protein tyrosine phosphatases. The cDNA sequence of human PTEN gene is presented. Also described are methods of diagnosis and treatment, e.g., of prostate cancer, utilizing compns. comprising PTEN or altered PTEN or nucleic acid mols. encoding PTEN or altered PTEN.
IT 203938-37-8
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(as substrate of phosphatase; dual specificity phosphatase PTEN and methods of use and structure of PTEN gene)
RN 203938-37-8 CAPLUS
CN myo-Inositol, 2-[4-[[5-(2-aminoethyl)-2-hydroxyphenyl]azo]benzoate] 1-[(2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] 3,4-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

L31 ANSWER 42 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PAGE 1-A



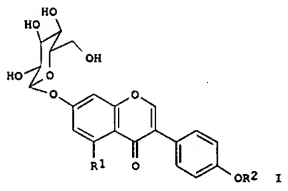
PAGE 1-B



L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:614289 CAPLUS
DOCUMENT NUMBER: 129:316503
TITLE: Preparation of unsaturated phosphatidylinositol polyphosphates using fluorenylmethyl group as phosphate-protecting group and intermediates therefor
INVENTOR(S): Watanabe, Hiroshi; Awaya, Akira
PATENT ASSIGNEE(S): Mitsui Pharmaceuticals, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 10251280 | A | 19980922 | JP 1997-74421 | 19970311 |
| PRIORITY APPLN. INFO.: | | | JP 1997-74421 | 19970311 |

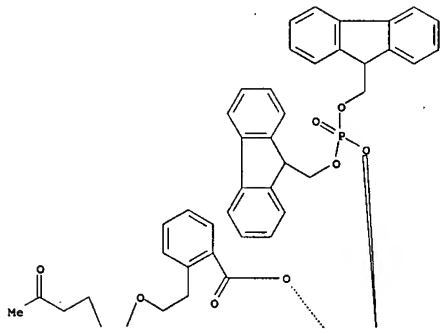
GI



AB The title compds., useful as tools for biochem. studies on polyphosphoinositides, are prepared Inositol phosphates, in which OH of sugar moiety is substituted with 2-[2-(levulinoyloxy)ethyl]benzoyl group and OH of phosphate moiety is protected with fluorenylmethyl, are also claimed. Preparation of 1-O-(1,2-di-O-oleoylglycerylphosphoryl)-3,4,5-tri-O-phosphoryl-myo-inositol from 1,2-O-cyclohexylidene-6-O-levulinoyl-myo-inositol and di-9-fluorenylmethyl N,N-Diisopropylphosphoramidite with 9 steps was given.
IT 214422-44-3P 214422-46-5P 214422-48-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of unsatd. phosphatidylinositol polyphosphates via protecting phosphate with fluorenylmethyl group)
RN 214422-44-3 CAPLUS
CN D-myo-Inositol, 4,5-bis[bis(9H-fluoren-9-ylmethyl) phosphate] 1-[(2R)-2,3-bis[[(9Z)-1-oxo-9-octadecenyl]oxy]propyl hydrogen phosphate] 3,6-bis[2-[2-[(1,4-dioxopentyl)oxy]ethyl]benzoate], monosodium salt (9CI) (CA INDEX NAME)

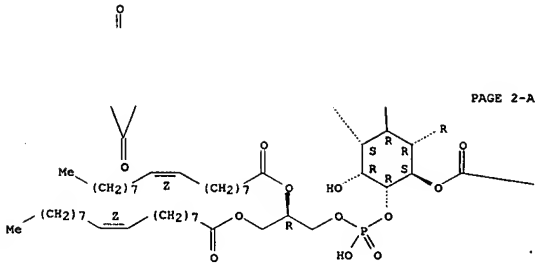
L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

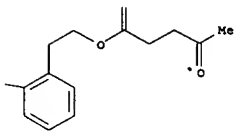


PAGE 2-A

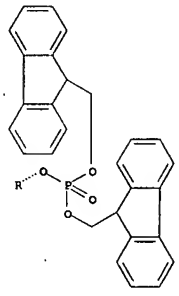


L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-B



PAGE 3-A



PAGE 3-B

● Na

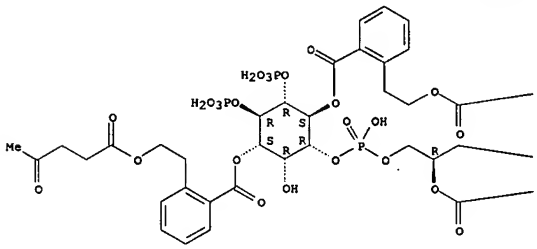
RN 214422-46-5 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis[[(9Z)-1-oxo-9-octadecenyl]oxy]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) 3,6-bis[2-[2-[(1,4-dioxopentyl)oxy]ethyl]benzoate], compd. with N,N-diethylethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

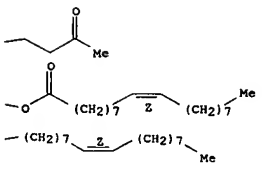
CRN 214422-45-4
CMF C73 H113 O27 P3

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



CM 2

CRN 121-44-8
CMF C6 H15 N

L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

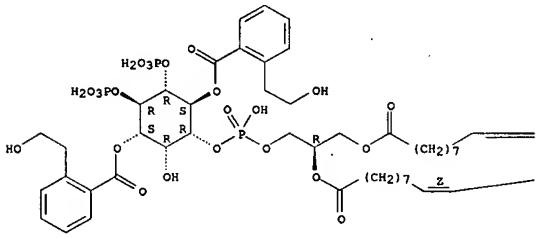
RN 214422-48-7 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis[[(9Z)-1-oxo-9-octadecenyl]oxy]propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) 3,6-bis[2-(2-hydroxyethyl)benzoate], monosodium salt, compd. with N,N-diethylethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 214422-47-6
CMF C63 H101 O23 P3

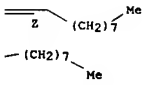
Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



L31 ANSWER 43 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



CM 2

CRN 121-44-8
CMF C6 H15 N

Previous O.A.

L31 ANSWER 44 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

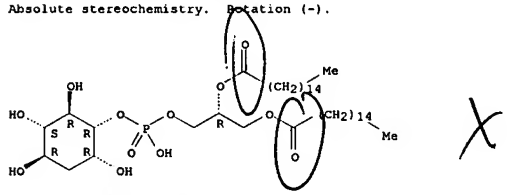
ACCESSION NUMBER: 1998:503329 CAPLUS
DOCUMENT NUMBER: 129:254488
TITLE: 3-Deoxy-D-myo-inositol 1-phosphate, 1-phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth
AUTHOR(S): Qiao, Lixin; Nan, Fajun; Kunkel, Mark; Gallegos, Alfred; Powis, Garth; Kozikowski, Alan P.
CORPORATE SOURCE: Drug Discovery Program, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(18), 3303-3306
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis and the bioactivity of several ratioally designed phosphatidylinositol analogs are presented. The studies have been directed toward the synthesis of 3-substituted myo-inositol derivs. to selectively block the effects of myo-inositol-derived second messengers on cell proliferation and transformation while living other aspects of myo-inositol signalling uneffected. This strategy may offer a basis for the selective control of cancer growth without disrupting the function of normal cells.

IT 162792-27-0P 213388-41-1P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyoinositol phosphate, phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol kinase signaling and cancer cell growth)

RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

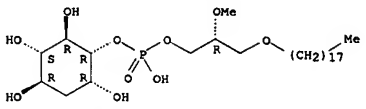
Absolute stereochemistry. Rotation (-).



RN 213388-41-1 CAPLUS
CN chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3R)-3-methoxy-4-(octadecyloxy)butyl]phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

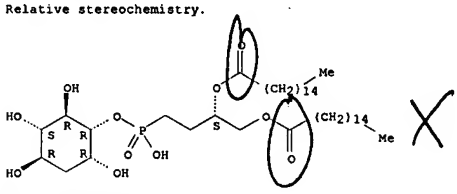
L31 ANSWER 44 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 213388-40-0P 213388-42-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyoinositol phosphate, phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol kinase signaling and cancer cell growth)

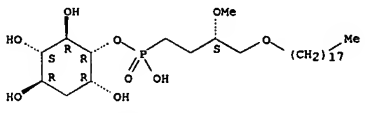
RN 213388-40-0 CAPLUS
CN D-chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3R)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate], rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 213388-42-2 CAPLUS
CN chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3S)-3-methoxy-4-(octadecyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

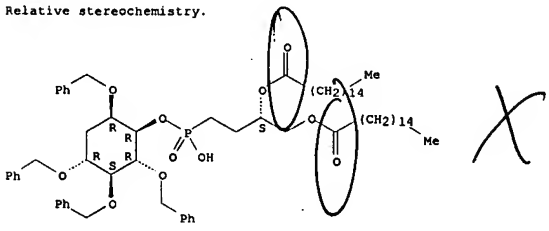


IT 213388-45-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(deoxymyoinositol phosphate, phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol kinase signaling and cancer cell growth)

RN 213388-45-5 CAPLUS
CN D-chiro-Inositol, 1-deoxy-2,3,4,6-tetrakis-O-(phenylmethyl)-, hydrogen

L31 ANSWER 44 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
[(3R)-3,4-bis[(1-oxohexadecyl)oxy]butyl]phosphonate, rel- (9CI) (CA INDEX NAME)

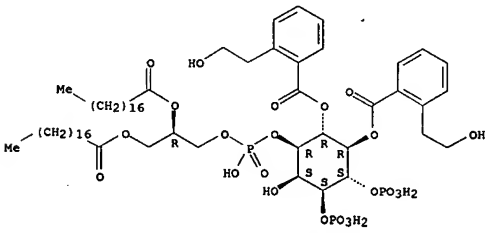
Relative stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 45 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:439297 CAPLUS
DOCUMENT NUMBER: 129:216836
TITLE: Synthesis of a distearoyl analog of phosphatidylinositol 3,4-bisphosphate
AUTHOR(S): Watanabe, Yutaka; Abe, Yoshinobu; Takao, Hiroyuki
CORPORATE SOURCE: Dep. Applied Chem., Fac. Eng., Ehime Univ., Matsuyama, 790-77, Japan
SOURCE: Carbohydrate Letters (1998), 3(2), 85-90
CODEN: CLETEC; ISSN: 1073-5070
PUBLISHER: Harwood Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Synthesis of the title compound was accomplished concisely via 1,2-cyclohexylidene-3,4-tetraisopropyldisiloxanyl-myo-inositol using a novel hydroxy protecting group and, selective and exhaustive phosphorylation methods which were all recently developed by us. The chiral synthesis was formally accomplished by kinetic resolution employing tartaroylation of a 1,2-diol derivative
IT 212326-19-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a distearoyl analog of phosphatidylinositol bisphosphate)
RN 212326-19-7 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] 3,4-bis(dihydrogen phosphate) 5,6-bis[2-(2-hydroxyethyl)benzoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

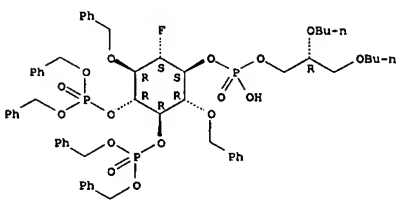


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 45 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L31 ANSWER 46 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:330471 CAPLUS
DOCUMENT NUMBER: 129:67941
TITLE: Synthesis of 2-deoxy-2-fluoro-phosphatidylinositol-4,5-bisphosphate and analogs: probes and modulators of the mammalian PI-PLCS
AUTHOR(S): Aneja, Sarla G.; Ivanova, Pavlina T.; Aneja, Rajindra
CORPORATE SOURCE: Functional Lipids Division, Langmuir Laboratory, Nutrimed Biotech, Cornell University Research Park, Ithaca, NY, 14850, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(9), 1061-1064
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An approach to synthesis of 2-modified phosphatidylinositol-4,5-bisphosphates, which are substrate analogs useful as probes and modulators of the PI-PLC enzyme family, is described and illustrated for the dibutyl-2-deoxy-2-fluoro analog, a probe designed for delineating substrate and PI-PLC interactions by X-ray crystallog.
IT 208844-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deoxyfluorophosphatidylinositol bisphosphate and analogs as probes and modulators of the mammalian PI-PLCS)
RN 208844-99-9 CAPLUS
CN D-scyllo-Inositol, 1-deoxy-1-fluoro-3,6-bis-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 2-[(2R)-2,3-dibutoxypropyl hydrogen phosphate] (9CI) (CA INDEX NAME)

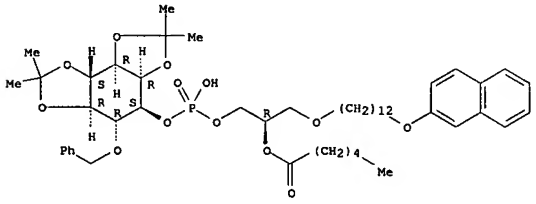
Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 47 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:307658 CAPLUS
DOCUMENT NUMBER: 129:28141
TITLE: Synthesis of fluorescent phosphatidylinositols using a novel inositol H-phosphonate
AUTHOR(S): Leung, Lawrence W.; Vilcheze, Catherine; Bittman, Robert
CORPORATE SOURCE: Dep. Chem. Biochem., Queens Coll. City Univ. New York, Flusing, NY, 11367-1597, USA
SOURCE: Tetrahedron Letters (1998), 39(19), 2921-2924
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Coupling of 1,2-diradyl-sn-glycerol with the novel inositol H-phosphonate derivative, 6-O-benzyl-2,3:4,5-di-O-isopropylidene-myo-inositol H-phosphonate, gave fluorescent analogs of phosphatidylinositol (PtdIns) and PtdIns(4,5)-bisphosphate (PtdIns(4,5)P2). Unlike the corresponding phosphoramidate, 6-O-benzyl-2,3:4,5-di-O-isopropylidene-myo-inositol H-phosphonate was stable at -20° for several months, making it a useful intermediate for the synthesis of myo-inositol phospholipids.
IT 207981-82-6P 207981-85-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent phosphatidylinositols using novel inositol H-phosphonate)
RN 207981-82-6 CAPLUS
CN D-myo-Inositol, 2,3:4,5-bis-O-(1-methylethylidene)-6-O-(phenylmethyl)-, (2R)-3-[[12-(2-naphthalenyloxy)dodecyl]oxy]-2-[(1-oxohexyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

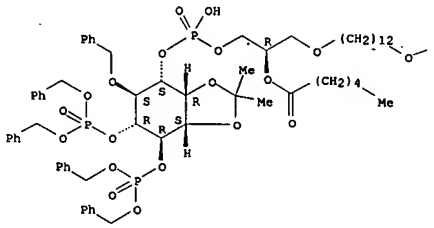


RN 207981-85-9 CAPLUS
CN D-myo-Inositol, 2,3-O-(1-methylethylidene)-6-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 1-[(2R)-3-[[12-(2-naphthalenyloxy)dodecyl]oxy]-2-[(1-oxohexyl)oxy]propyl hydrogen phosphate]

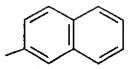
L31 ANSWER 47 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

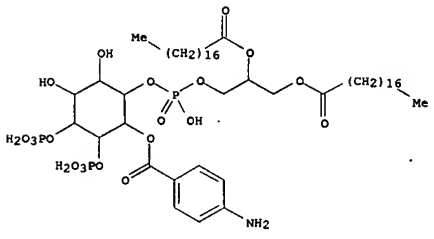


PAGE 1-B



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 48 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:138448 CAPLUS
DOCUMENT NUMBER: 128:205067
TITLE: Synthesis of affinity column of phosphatidylinositol-3,4-diphosphate
AUTHOR(S): Ozaki, Shoichiro; Kong, Xiang-Zheng; Watanabe, Yutaka; Ogasawara, Tomio
CORPORATE SOURCE: Department of Chemistry, Shandong University, Jinan, 250100, Peop. Rep. China
SOURCE: Chinese Journal of Chemistry (1997), 15(6), 556-561
CODEN: CJOCEV; ISSN: 1001-604X
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phosphatidylinositol polyphosphates (PIPx) are related with tyrosine kinase activation, cell proliferation and carcinogenesis. In order to investigate the action mechanism of PIPx, it is desirable to synthesize affinity column of PI-3,4-P2, which is expected to be able to isolate the binding proteins of PI-3,4-P2. Tyramine reacted with CH-Sepharose 4B giving column 13. The p-amino group of 3'-(1',2'-distearoyl-glyceryl)-1-(2-p-aminobenzyl)-3,4-di-O-phosphoryl-myo-inositol phosphate (I) was diazotized, then diazo-coupled with column 13 to give PI-3,4-P2 affinity column 14. This PI-3,4-P2 affinity column is an effective tool to pick up binding proteins of PI-3,4-P2.
IT 203938-36-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of affinity column of phosphatidylinositol-3,4-diphosphate)
RN 203938-36-7 CAPLUS
CN myo-Inositol, 2-(4-aminobenzoate) 1-[(2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] 3,4-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

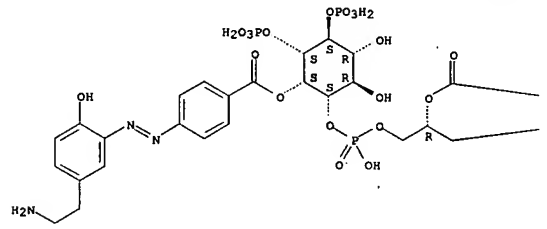


IT 203938-37-8DP, CH-Sepharose 4B bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of affinity column of phosphatidylinositol-3,4-diphosphate)
RN 203938-37-8 CAPLUS
CN myo-Inositol, 2-[4-[[5-(2-aminoethyl)-2-hydroxyphenyl]azo]benzoate] 1-[(2R)-2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate]

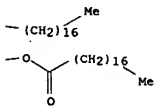
L31 ANSWER 48 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
3,4-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

PAGE 1-A

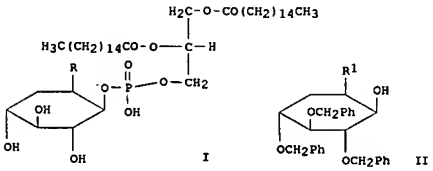


PAGE 1-B



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L31 ANSWER 49 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:714361 CAPLUS
DOCUMENT NUMBER: 127:359017
TITLE: Synthesis of 1D-3-deoxy- and -2,3-dideoxyphosphatidylinositol
AUTHOR(S): Kozikowski, Alan P.; Qiao, Lixin; Tuckmantel, Werner; Powis, Garth
CORPORATE SOURCE: Institute of Cognitive and Computational Sciences, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Tetrahedron (1997), 53(44), 14903-14914
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

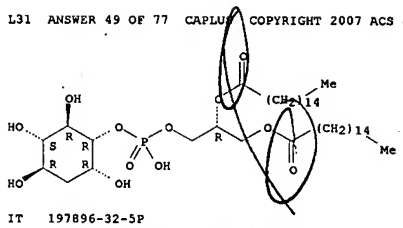


I II

AB Both 1D-3-deoxy- and -2,3-dideoxyphosphatidylinositol (I, R = OH, H) were synthesized using the regioisomeric mixture of viburnitol 1,2:4,5- and 1,2:5,6- diacetonides as starting material. Selective acidic hydrolysis and subsequent benzylation or deoxygenation afforded II (R1 = OCH2Ph, H) as important intermediates. Compds. I were of interest as putative antimetabolites of phosphatidylinositol-3-phosphate and as inhibitors of cancer cell colony formation.
IT 162792-27-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of 1D-3-deoxy- and -2,3-dideoxyphosphatidylinositol)
RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

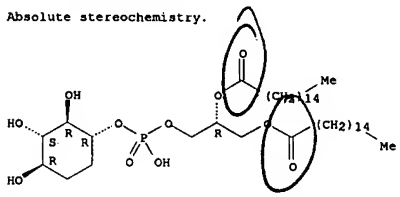
Absolute stereochemistry. Rotation (-).

L31 ANSWER 49 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 197896-32-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 1D-3-deoxy- and -2,3-dideoxyphosphatidylinositol)
RN 197896-32-5 CAPLUS
CN Hexadecanoic acid, (1R)-1-[[[hydroxy[[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl]oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

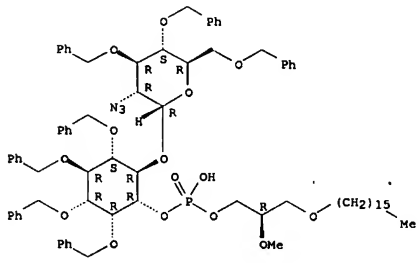
L31 ANSWER 50 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:663354 CAPLUS
DOCUMENT NUMBER: 127:307581
TITLE: Parasite glycoconjugates. Part 7. Synthesis of further
substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors
AUTHOR(S): Crossman, Arthur, Jr.; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: Department of Chemistry, University of Dundee, Dundee,
DD1 4HN, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (18), 2769-2774
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Substrate analogs of 1D-6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-[sn-2,3-bis(myristoyloxy)propyl phosphate], an early intermediate in the bio-preparation of glycosylphosphatidylinositol (GPI) membrane anchors, have been prepared for biol. evaluation with the α-(1→4)-D-mannosyltransferase of the protozoan parasite Trypanosoma brucei. The analog α-D-GlcpNH2-(1→6)-2-OMe-PI is a substrate for the protozoan α-(1→4)-D-mannosyltransferase but not for the corresponding mammalian enzyme, whereas the analogs, in which the fatty-acid groups of the natural substrate are replaced by alkyl
groups, are acceptable substrates for both the protozoan and mammalian enzymes.
IT 197369-86-1P 197369-88-3P 197385-16-3P
197385-17-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of glycosylphosphatidylinositol membrane anchors as substrates
for the protozoan mannosyltransferase)
RN 197369-86-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 197369-85-0
CMF C81 H104 N3 O15 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 50 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

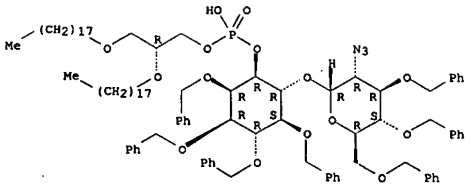
RN 197369-88-3 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 197369-87-2
CMF C100 H142 N3 O15 P

Absolute stereochemistry. Rotation (+).

L31 ANSWER 50 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

RN 197385-16-3 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

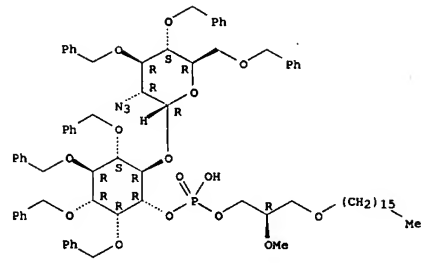
Absolute stereochemistry. Rotation (+).

L31 ANSWER 50 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 50 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

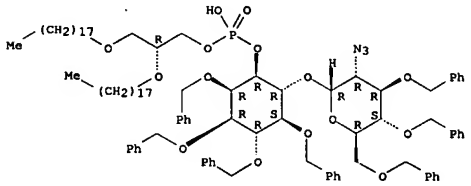


PAGE 2-A

● Na

RN 197385-17-4 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-(octadecyloxy)propyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

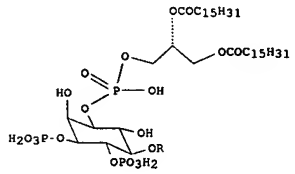
Absolute stereochemistry. Rotation (+).



● Na

L31 ANSWER 51 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:621264 CAPLUS
DOCUMENT NUMBER: 127:262942
TITLE: Synthesis of dipalmitoyl phosphatidylinositol 3,4-bis(phosphate) and 3,4,5-tris(phosphate) and their enantiomers
AUTHOR(S): Grove, Simon J. A.; Holmes, Andrew B.; Painter, Gavin F.; Hawkins, Phillip T.; Stephens, Leonard R.
CORPORATE SOURCE: Cambridge Centre for Molecular Recognition, Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK
SOURCE: Chemical Communications (Cambridge) (1997), (17), 1635-1639
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

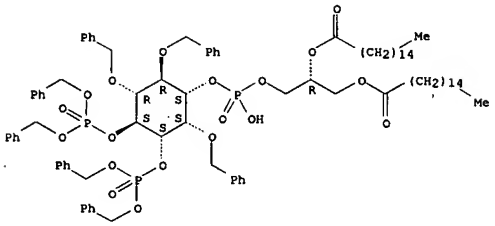
AB The dipalmitoyl phosphatidylinositol phosphates I (R = H, PO3H2) and their enantiomers are synthesized from homochiral myo-inositol precursors.

IT 196304-59-3P 196304-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dipalmitoyl phosphatidylinositol 3,4-bis(phosphate) and 3,4,5-tris(phosphate) and their enantiomers)

RN 196304-59-3 CAPLUS
CN D-myo-Inositol, 2,5,6-tris-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3,4-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

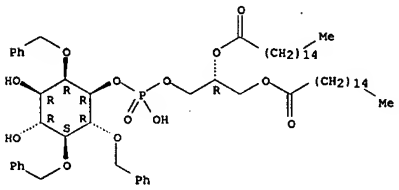
Absolute stereochemistry. Rotation (+).

L31 ANSWER 51 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



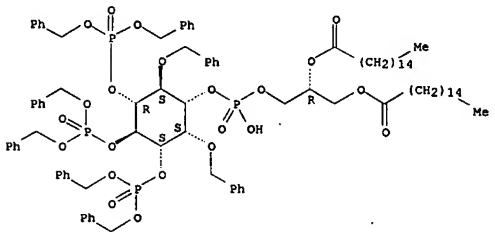
RN 196304-64-0 CAPLUS
CN D-myo-Inositol, 2,5,6-tris-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



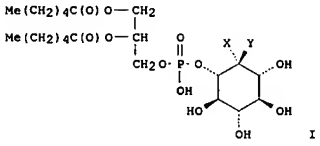
L31 ANSWER 52 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:106429 CAPLUS
DOCUMENT NUMBER: 126:212332
TITLE: A unified approach to unambiguous synthesis of the phosphatidylinositol-3-phosphates involved in intracellular signal transduction
AUTHOR(S): Aneja, Sarla G.; Parra, Alejandro; Stoenescu, Caterina; Xia, Wenyu; Aneja, Rajindra
CORPORATE SOURCE: Langmuir Laboratory, Cornell Univ. Res. Park, Ithaca, NY, 14850, USA
SOURCE: Tetrahedron Letters (1997), 38(5), 803-806
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:212332
AB A unified approach to unambiguous preparation of the phosphatidylinositol-3-phosphates involved in intracellular signaling is illustrated by the preparation of 1D-1-(1',2'-dihexadecanoyl-sn-glycero-3'-phospho)-myo-inositol-3,4,5-triphosphate.
IT 188112-77-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phosphatidylinositol phosphates)
RN 188112-77-8 CAPLUS
CN D-myo-Inositol, 2,6-bis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] 3,4,5-tris(bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 53 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:650029 CAPLUS
DOCUMENT NUMBER: 126:3591
TITLE: Synthesis and Kinetic Evaluation of Inhibitors of the Phosphatidylinositol-Specific Phospholipase C from Bacillus cereus
AUTHOR(S): Martin, Stephen F.; Wagman, Allan S.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA
SOURCE: Journal of Organic Chemistry (1996), 61(23), 8016-8023
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:3591
GI

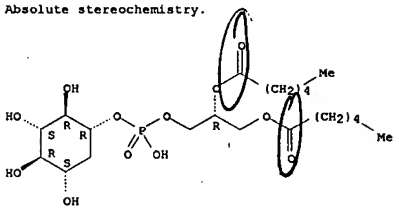


I

AB Substrate analogs of phosphatidylinositol were synthesized and evaluated as potential inhibitors of the bacterial phosphatidylinositol-specific phospholipase C (PI-PLC) from Bacillus cereus. The chiral analogs of the water-soluble phospholipid substrate (I) were designed to probe the effects of varying the inositol C-2 hydroxyl group, which is generally believed to serve as the nucleophile in the first step of the hydrolysis of phosphatidylinositols by PI-PLC. In the analogs, the C-2 hydroxyl group on the inositol ring of the phosphatidylinositol derivs. was rationally altered in several ways. Inversion of the stereochem. at C-2 of the inositol ring led to the scyllo derivative The inositol C-2 hydroxy group was replaced with inversion by a fluorine to produce the scyllo-fluoro inositol and with a hydrogen atom to furnish the 2-deoxy compound The C-2 hydroxyl group was O-methylated to prepare the methoxy derivative The natural inositol configuration at C-2 was retained in the nonhydrolyzable phosphorodithioate analog. The inhibition of PI-PLC by each of these analogs was then analyzed in a continuous assay using D-myo-inositol 1-(4-nitrophenyl phosphate) as a chromogenic substrate. The kinetic parameters for each of these phosphatidylinositol derivs. were determined, and each was found to be a competitive inhibitor. This study further establishes that the hydrolysis of phosphatidylinositol analogs by bacterial PI-PLC requires not only the presence of a C-2 hydroxyl group on

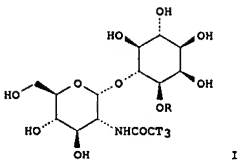
L31 ANSWER 53 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
the inositol ring, but the stereochem. at this position must also correspond to the natural myo-configuration. For future inhibitor design, it is perhaps noteworthy that the best inhibitors possess a hydroxyl group at the C-2 position. Several of the inhibitors identified in this study are now being used to obtain crystallog. information for an enzyme-inhibitor complex to gain further insights regarding the mechanism of hydrolysis of phosphatidylinositides by this PI-PLC.
IT 183447-80-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(synthesis and kinetic evaluation of inhibitors of the phosphatidylinositol-specific phospholipase C from Bacillus cereus)
RN 183447-80-5 CAPLUS
CN D-myo-Inositol, 2-deoxy-, 1-[(2R)-2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:692419 CAPLUS
DOCUMENT NUMBER: 124:30178
TITLE: Parasite glycoconjugates. Part 3. Synthesis of substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors
AUTHOR(S): Cottaz, Sylvain; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, DD1 4HN, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (13), 1673-8
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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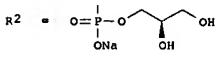
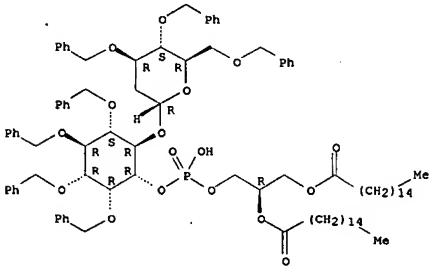


AB Substrate analogs of sodium 1D-6-O-[2-[3H3]acetamido-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-[sn-2,3-bis(palmitoyloxy)propyl phosphate], including the lipid-depleted compds., e.g. I (R = H, PO3H2, R2), have been prepared for biol. evaluation with a partially purified de-N-acetylase from the bloodstream form of the parasitic protozoan Trypanosoma brucei.

IT 154372-22-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of substrate analogs of glycosylphosphatidylinositol membrane anchors as deacetylase inhibitors)

RN 154372-22-2 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 121-44-8
CMF C6 H15 N

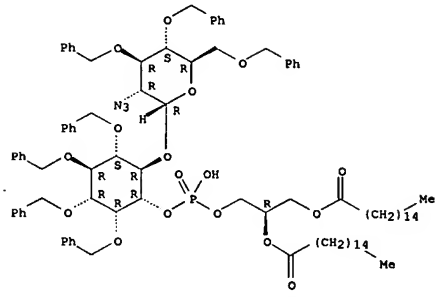
RN 171482-45-4 CAPLUS
CN D-myo-Inositol, 2,3,4,5-tetrakis-O-(phenylmethyl)-6-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, monosodium salt, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 786618-74-4
CMF C103 H137 O18 P

Absolute stereochemistry.

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.



IT 171283-64-0P 171482-45-4P 171482-46-5P
171482-47-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of substrate analogs of glycosylphosphatidylinositol membrane anchors as deacetylase inhibitors)

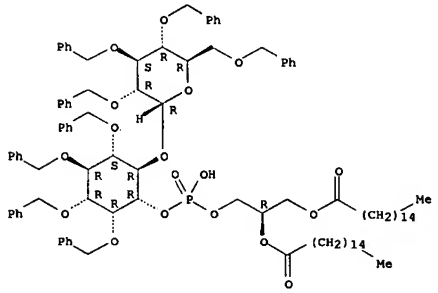
RN 171283-64-0 CAPLUS
CN D-myo-Inositol, 6-O-[2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-arabino-hexopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171283-63-9
CMF C96 H131 O17 P

Absolute stereochemistry.

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

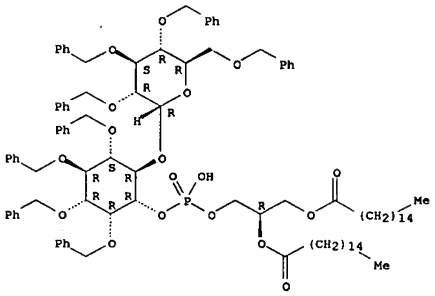
CRN 121-44-8
CMF C6 H15 N

RN 171482-46-5 CAPLUS
CN D-myo-Inositol, 2,3,4,5-tetrakis-O-(phenylmethyl)-6-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

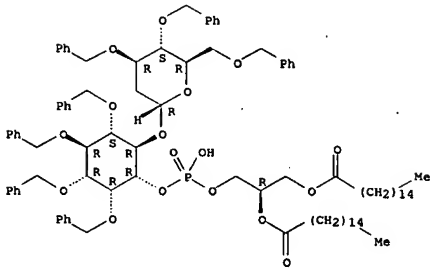
● Na

RN 171482-47-6 CAPLUS
CN D-myo-Inositol, 6-O-[2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-arabino-hexopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 54 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

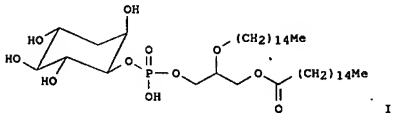


PAGE 2-A

● Na

L31 ANSWER 55 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:448576 CAPLUS
DOCUMENT NUMBER: 122:291368
TITLE: Synthesis and Biology of 1D-3-Deoxyphosphatidylinositol: A Putative Antimetabolite of Phosphatidylinositol-3-phosphate and an Inhibitor of Cancer Cell Colony Formation
AUTHOR(S): Kozikowski, Alan P.; Kiddle, James J.; Frew, Timothy; Berggren, Margareta; Powis, Garth
CORPORATE SOURCE: Neurochemistry Research, Princeton, NJ, 08540, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(7), 1053-6
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

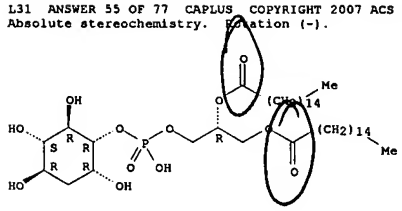
AB A total synthesis of the novel 3-deoxy analog of phosphatidylinositol (PtdIns) is reported. The previously synthesized precursor 1D-4-benzyl-3-deoxy-5,6-dibenzoyl-1,2-O-isopropylidene-myo-inositol derived from L-quebrachitol, serves as the starting material for the synthesis of 1D-3-deoxyphosphatidylinositol I. Manipulation of this compound to bring about selective benzylation of all hydroxyl groups but the 1-OH, to which the phosphatidic acid side chain is attached via phosphoramidite chemical, followed by deprotection to give the title compound is presented. I is shown to be an effective inhibitor of the colony formation of HT-29 colon cancer cells with an IC50 of 35 μM. I is not a substrate for PtdIns-3-kinase, nor does it inhibit PtdIns-3-kinase activity. This novel analog may thus act as an antimetabolite of phosphatidylinositol-3-phosphate. I can also be used to measure PtdIns-3-kinase activity in diverse cell lines. The biol. activity found for this compound provides further support for the pursuit of a PtdIns-based approach to the discovery of potential anticancer agents.

IT 162792-27-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. of deoxyphosphatidylinositol a putative antimetabolite of phosphatidylinositolphosphate and an inhibitor of cancer cell colony formation)

RN 162792-27-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-, 5-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L31 ANSWER 55 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry. Rotation (-).



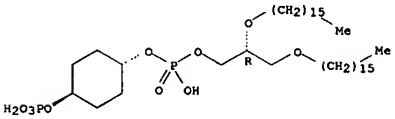
L31 ANSWER 56 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:100000 CAPLUS
DOCUMENT NUMBER: 122:127265
TITLE: Inhibition of human erythrocyte membrane phosphatidylinositol 4-kinase by phospholipid analogs
AUTHOR(S): Young, R. C.; Downes, C. P.; Jones, M.; Milliner, K. J.; Rana, K. K.; Ward, J. G.
CORPORATE SOURCE: SmithKline Beecham Pharmaceuticals, Welwyn/Hertfordshire, AL6 9AR, UK
SOURCE: European Journal of Medicinal Chemistry (1994), 29(7-8), 537-49
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Analogs of phosphatidylinositol (PtdIns, 1) have been synthesized to investigate the structural requirements for inhibition of a PtdIns 4-kinase obtained from human erythrocyte membranes. While the presence of either D-1 or D-3 stereochem. in the inositol moiety greatly influences the degree of inhibition produced by PtdIns analogs, the stereochem. of the glycerol moiety is of little consequence. Neither structural feature, however, makes a significant contribution to binding affinity. Competitive inhibitory activity was retained (or even enhanced) in substantially simpler analogs consisting of 1 or 2 hydrocarbon chains attached to a charged phosphate head group, such as in the phosphatidic acids. The observation that the phosphatidylinositol 4-phosphate (PtdIns 4P) and phosphatidic acid analogs inhibit PtdIns 4-kinase may suggest that such species have a regulatory role in PtdIns turnover.

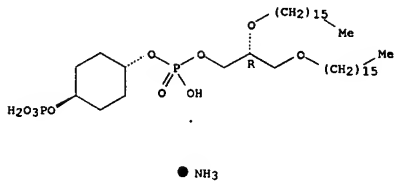
IT 161105-07-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of phospholipid analogs and evaluation as phosphatidylinositol 4-kinase inhibitors)
RN 161105-07-3 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono[4-(phosphonooxy)cyclohexyl] ester, monoammonium salt, [1(R)-trans]- (9CI) (CA INDEX NAME)

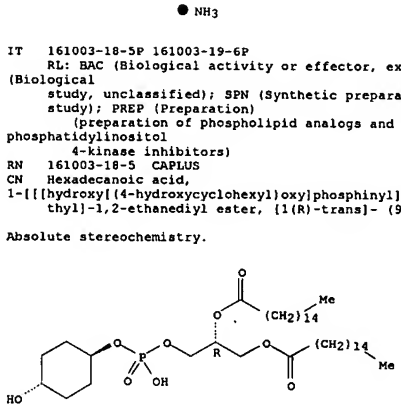
Absolute stereochemistry.

L31 ANSWER 56 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L31 ANSWER 56 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)





IT 161003-18-5P 161003-19-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of phospholipid analogs and evaluation as phosphatidylinositol 4-kinase inhibitors)
RN 161003-18-5 CAPLUS
CN Hexadecanoic acid, 1-[[[hydroxy[(4-hydroxycyclohexyl)oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester, [1(R)-trans]- (9CI) (CA INDEX NAME)

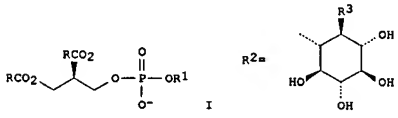
Absolute stereochemistry.



RN 161003-19-6 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono[4-(phosphonooxy)cyclohexyl] ester, [1(R)-trans]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 57 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:21799 CAPLUS
DOCUMENT NUMBER: 122:106298
TITLE: General Method for the Synthesis of Phospholipid Derivatives of 1,2-O-Diacyl-sn-Glycerols
AUTHOR(S): Martin, Stephen F.; Josey, John A.; Wong, Yue-Ling; Dean, Daniel W.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA
SOURCE: Journal of Organic Chemistry (1994), 59(17), 4805-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:106298
GI

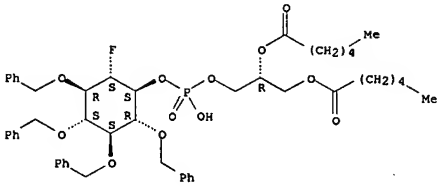


AB An efficient phosphite coupling protocol is described for the syntheses of the major classes of glycerophospholipids, e.g. I [R = (CH2)4Me, R1 = (CH2)2NH3+, R2; R3 = H, F, OH], that are derived from 1,2-O-diacyl-sn-glycerols and analogs thereof. This phosphite coupling procedure was modified to assemble phospholipids bearing polyunsatd. acyl side chains at the sn-2-position as exemplified by the preparation of the phosphatidylethanolamine. The one-pot phosphite coupling procedure is also applicable to the syntheses of a variety of other biol. interesting phospholipid analogs.

IT 160531-77-1P 160531-78-2P 160531-79-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 160531-77-1 CAPLUS
CN D-scyllo-Inositol, 1-deoxy-1-fluoro-3,4,5,6-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate, (R)- (9CI) (CA INDEX NAME)

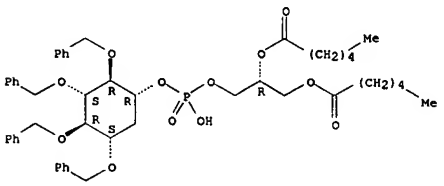
Absolute stereochemistry.

L31 ANSWER 57 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 160531-78-2 CAPLUS
CN D-myo-Inositol, 2-deoxy-3,4,5,6-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate, (R)- (9CI) (CA INDEX NAME)

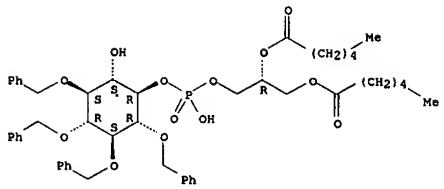
Absolute stereochemistry.



RN 160531-79-3 CAPLUS
CN D-scyllo-Inositol, 1,2,3,4-tetrakis-O-(phenylmethyl)-, 5-[2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate], (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 57 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L31 ANSWER 58 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:270999 CAPLUS
DOCUMENT NUMBER: 120:270999
TITLE: Parasite glycoconjugates. Part 1. The synthesis of some early and related intermediates in the biosynthetic pathway of glycosyl-phosphatidylinositol membrane anchors
AUTHOR(S): Cottaz, Sylvain; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, DD1 4HN, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (23), 2945-51
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The enantio-pure 1D- and 1L-myo-inositol deriva. I have been used to prepare sodium (aminodeoxy-α-D-glucopyranosyl)-myo-inositol phosphate II and a related 1,6-disubstituted 1L-myo-inositol III. The hydrogenphosphonate approach was effective in coupling together the phosphonolipid moiety and the protected 6-O-(2-azido-2-deoxy-α-D-glucopyranosyl)-myo-inositols.

IT 154372-23-3P 154459-87-7P 154459-91-3P
154568-19-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in preparation of glycosylphosphatidylinositol)

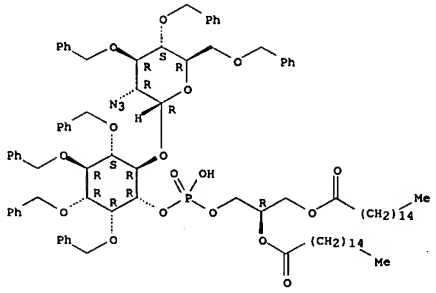
RN 154372-23-3 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 154372-22-2
CMF C96 H130 N3 O17 P

Absolute stereochemistry.

L31 ANSWER 58 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

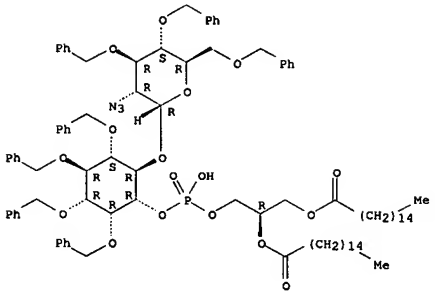
CRN 121-44-8
CMF C6 H15 N

RN 154459-87-7 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 58 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



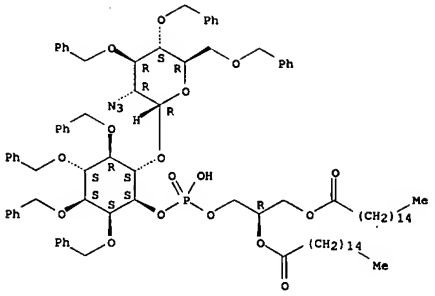
PAGE 2-A

● Na

RN 154459-91-3 CAPLUS
CN D-myo-Inositol, 4-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-1,2,5,6-tetrakis-O-(phenylmethyl)-, 3-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 58 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



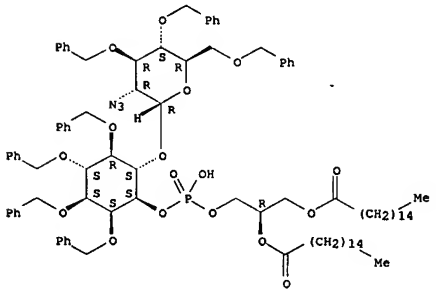
RN 154568-19-1 CAPLUS
CN D-myo-Inositol, 4-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-1,2,5,6-tetrakis-O-(phenylmethyl)-, 3-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 154459-91-3
CMF C96 H130 N3 O17 P

Absolute stereochemistry.

L31 ANSWER 58 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

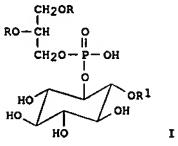


CM 2

CRN 121-44-8
CMF C6 H15 N

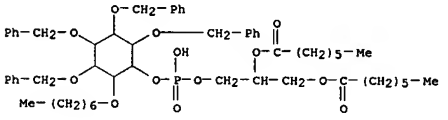
L31 ANSWER 59 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:164723 CAPLUS
DOCUMENT NUMBER: 120:164723
TITLE: Synthesis of phosphatidyl-2-O-alkylinositols as potential inhibitors for PI specific PLC
AUTHOR(S): Garigapati, Venkata R.; Roberts, Mary F.
CORPORATE SOURCE: Dep. Chem., Boston College, Chestnut Hill, MA, 02154, USA
SOURCE: Tetrahedron Letters (1993), 34(35), 5579-82
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



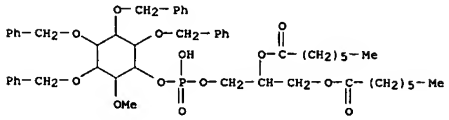
I

AB (±)-Racemic phosphatidyl-2-O-methylinositol and phosphatidyl-2-O-heptylinositol I [R = CO(CH2)5Me, R1 = Me, (CH2)6Me] were synthesized and tested as mechanism-based inhibitors of bacterial PI-PLC activity.
IT 153237-85-5P 153323-83-2P .
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in preparation of phosphatidylinositols)
RN 153237-85-5 CAPLUS
CN myo-Inositol, 2-O-heptyl-1,4,5,6-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxoheptyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)



RN 153323-83-2 CAPLUS
CN myo-Inositol, 2-O-methyl-1,4,5,6-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxoheptyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

L31 ANSWER 59 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



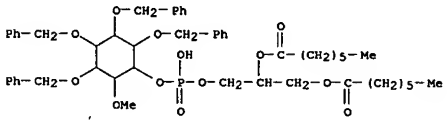
L31 ANSWER 60 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:3312 CAPLUS
DOCUMENT NUMBER: 120:3312
TITLE: Substrate requirements of bacterial phosphatidylinositol-specific phospholipase C
AUTHOR(S): Lewis, Karen A.; Garigapati, Venkata R.; Zhou, Chun; Roberts, Mary F.
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA
SOURCE: Biochemistry (1993), 32(34), 8836-41
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of sym. short-chain phosphatidylinositols (PI), including dihexanoyl-PI, diheptanoyl-PI (racemic as well as D and L forms), and 2-methoxyinositol-substituted heptanoyl-PI, were synthesized, characterized, and used to investigate key mechanistic questions about phosphatidylinositol phospholipase C (PI-PLC) from Bacillus thuringiensis.

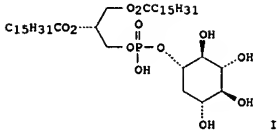
Key results included the following: (1) bacterial PI-PLC exhibited a 5-6-fold interfacial activation when its substrate was present in an interface as opposed to existing as a monomer in solution (in fact, the similarity to the activation observed with nonspecific PLC enzymes suggested a similarity in activation mechanisms); (2) the 2-OH group must be free since the enzyme could not hydrolyze diheptanoyl-2-O-methyl-PI (this was most consistent with the formation of inositol cyclic 1,2-phosphate as a necessary step in catalysis); (3) the inositol ring must have the D stereochem. (the L-inositol attached to the lipid moiety was neither a substrate nor an inhibitor); and (4) the presence of noninhibitory L-PI with the D-PI substrate relieved the diacylglycerol product inhibition detected at .apprx.30% hydrolysis.

IT 151555-15-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 151555-15-6 CAPLUS
CN D-myo-Inositol, 2-O-methyl-3,4,5,6-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxoheptyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



L31 ANSWER 61 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:539635 CAPLUS
DOCUMENT NUMBER: 119:139635
TITLE: Synthesis and enzymic properties of a deoxy analog of phosphatidylinositol
AUTHOR(S): Seitz, Steven P.; Kaltenbach, Robert F., III; Vreekamp, Remko H.; Calabrese, Joseph C.; Perrella, Frank W.
CORPORATE SOURCE: Cent. Res. Dep., Du Pont Merck Pharm. Co., Wilmington, DE, 19880, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1992), 2(2), 171-4
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:139635
GI

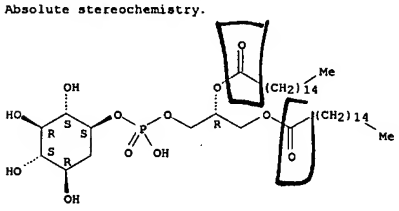


I

AB The preparation of a phosphatidylinositol analog I lacking the axial 2-hydroxyl of the inositol ring is described. The compound is a useful mechanistic probe for the phosphatidylinositol specific phospholipase C.

IT 149578-27-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of phospholipase C by)
RN 149578-27-8 CAPLUS
CN D-myo-Inositol, 2-deoxy-, 3-[(2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

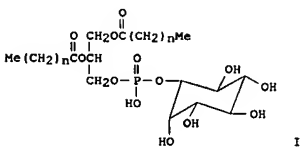
Absolute stereochemistry.



L31 ANSWER 61 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

$R^7$ = esters
$R^1$ =

L31 ANSWER 62 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:495985 CAPLUS
DOCUMENT NUMBER: 119:95985
TITLE: Synthesis of short chain phosphatidylinositols
AUTHOR(S): Garigapati, Venkata R.; Roberts, Mary F.
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA
SOURCE: Tetrahedron Letters (1993), 34(5), 769-72
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:95985
GI

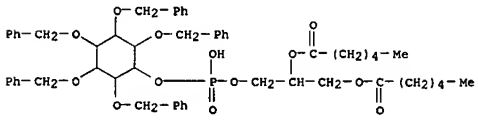


I

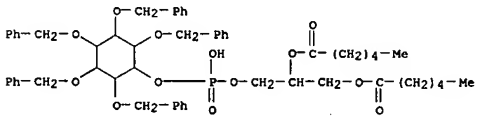
AB A short, convenient, and versatile synthesis of short chain D- and L-phosphatidylinositols, e.g. I (n = 4, 5) is reported.
IT 148437-38-1P 148437-40-5P 148553-35-9P
148553-37-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 148437-38-1 CAPLUS
CN D-myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 148437-37-0
CMF C56 H69 O13 P



L31 ANSWER 62 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



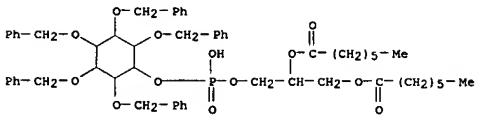
CM 2

CRN 121-44-8
CMF C6 H15 N

RN 148553-37-1 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxoheptyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine
(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 148553-36-0
CMF C58 H73 O13 P



CM 2

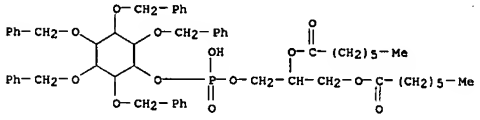
CRN 121-44-8
CMF C6 H15 N

L31 ANSWER 62 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 148437-40-5 CAPLUS
CN D-myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxoheptyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine
(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 148437-39-2
CMF C58 H73 O13 P



CM 2

CRN 121-44-8
CMF C6 H15 N

RN 148553-35-9 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxohexyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine
(1:1) (9CI) (CA INDEX NAME)

CM 1

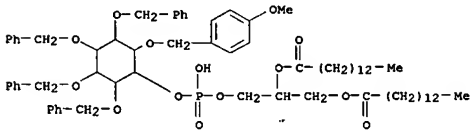
CRN 148553-34-8
CMF C56 H69 O13 P

L31 ANSWER 62 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L31 ANSWER 63 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:102344 CAPLUS
DOCUMENT NUMBER: 118:102344
TITLE: Synthetic studies on cell surface glycans. Part 83. Stereoselective synthesis of glycobiosyl phosphatidylinositol, a part structure of the glycosylphosphatidylinositol (GPI) anchor of Trypanosoma brucei
AUTHOR(S): Murakata, Chikara; Ogawa, Tomoya
CORPORATE SOURCE: RIKEN, Wako, 351-01, Japan
SOURCE: Carbohydrate Research (1992), 234, 75-91
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB O-α-D-Mannopyranosyl-(1→4)-O-2-amino-2-deoxy-α-D-glucopyranosyl-(1→6)-1D-myo-inositol 1-(1,2-di-O-myristoyl-sn-glycer-3-yl hydrogen phosphate), a part structure of the glycosylphosphatidylinositol anchor of T. brucei, was synthesized efficiently by the phosphonate approach. The glycobiosylinositol core was prepared in a stereocontrolled manner from 1D-2,3,4,5-tetra-O-benzyl-1-O-(4-methoxybenzyl)-myo-inositol, tert-butyldimethylsilyl 2-azido-3,6-di-O-benzyl-2-deoxy-α-D-glucopyranoside, and Me 3,6-di-O-acetyl-2,6-di-O-benzyl-2-thio-α-D-mannopyranoside.
IT 144733-50-6P 146076-24-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 144733-50-6 CAPLUS
CN D-myo-Inositol, 6-O-[(4-methoxyphenyl)methyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

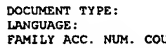
CM 1

CRN 144733-49-3
CMF C73 H103 O14 P



CM 2

CRN 121-44-8
CMF C6 H15 N

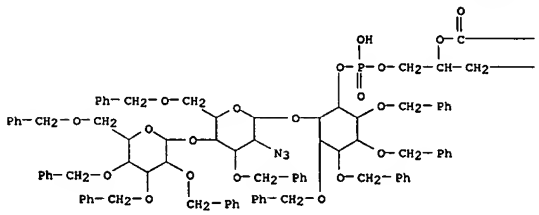


L31 ANSWER 63 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

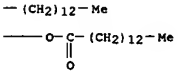


RN 146076-24-6 CAPLUS
CN D-myo-Inositol, O-2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl-(1→4)-O-2-azido-2-deoxy-3,6-bis-O-(phenylmethyl)-α-D-glucopyranosyl-(1→6)-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L31 ANSWER 64 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:22543 CAPLUS
DOCUMENT NUMBER: 118:22543
TITLE: Preparation of intermediates for glycosylphosphatidylinositol anchors
INVENTOR(S): Ogawa, Tomoya; Muragata, Tsutomu; Saito, Hiromitsu
PATENT ASSIGNEE(S): Institute of Physical and Chemical Research, Japan; Kyowa Hakko Kogyo Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 04120089 | A | 19920421 | JP 1990-240960 | 19900911 |
| PRIORITY APPLN. INFO.: | | | JP 1990-240960 | 19900911 |

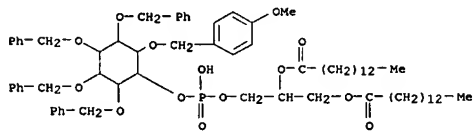
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title intermediates, e.g. I and II, are prepared E.g., I was prepared in 4 steps from the protected hexopyranose diacetate III via reaction with p-MeOC6H4OH in methylene chloride containing CF3SO3SiMe3, hydrolysis, reaction with benzyl alc., ClP[N(CHMe2)2]2, and HOCH2CH2NHCO2CH2Ph, and debenzylation.
IT 144733-50-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 144733-50-6 CAPLUS
CN D-myo-Inositol, 6-O-[(4-methoxyphenyl)methyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 144733-49-3
CMF C73 H103 O14 P



L31 ANSWER 64 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

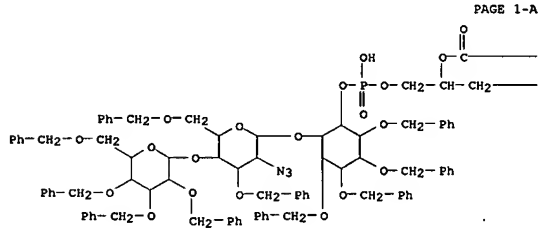
CM 2

CRN 121-44-8
CMF C6 H15 N

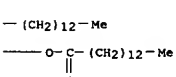


IT 132990-92-2P 144675-54-7P 144733-53-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of intermediates for glycosylphosphatidylinositol anchors)
RN 132990-92-2 CAPLUS
CN D-myo-Inositol, O-2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl-(1→4)-O-2-azido-2-deoxy-3,6-bis-O-(phenylmethyl)-α-D-glucopyranosyl-(1→6)-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate], (S)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

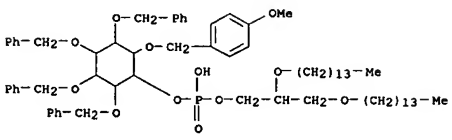


RN 144675-54-7 CAPLUS
CN D-myo-Inositol, 6-O-[(4-methoxyphenyl)methyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis(tetradecyloxy)propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

L31 ANSWER 64 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 144675-53-6
CMF C73 H107 O12 P



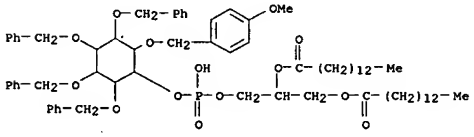
CM 2

CRN 121-44-8
CMF C6 H15 N

RN 144733-53-9 CAPLUS
CN D-myo-Inositol, 4-O-[(4-methoxyphenyl)methyl]-1,2,5,6-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 144733-52-8
CMF C73 H103 O14 P



CM 2

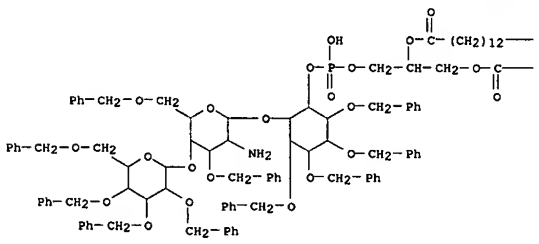
CRN 121-44-8

L31 ANSWER 64 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CMF C6 H15 N

IT 144675-55-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for glycosylphosphatidylinositol anchors)
RN 144675-55-8 CAPLUS
CN D-myo-Inositol, O-2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl-(1→4)-O-2-amino-2-deoxy-3,6-bis-O-(phenylmethyl)-α-D-glucopyranosyl-(1→6)-2,3,4,6-tetrakis-O-(phenylmethyl)-, 1-[2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



● Na

PAGE 1-B

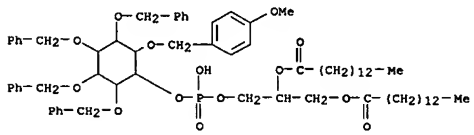
— Me

— $(CH_2)_{12}$ — Me

L31 ANSWER 64 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L31 ANSWER 65 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

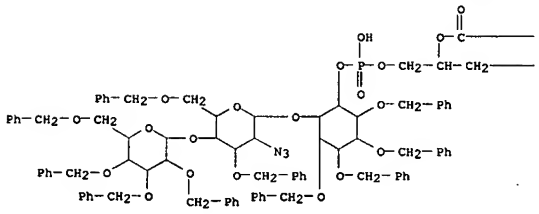
ACCESSION NUMBER: 1991:164666 CAPLUS
DOCUMENT NUMBER: 114:164666
TITLE: Synthetic studies on cell-surface glycans. 77. Synthetic studies on glycophosphatidylinositol anchor: a highly efficient synthesis of glycobiosyl phosphatidylinositol through H-phosphonate approach
AUTHOR(S): Murakata, Chikara; Ogawa, Tomoya
CORPORATE SOURCE: Inst. Phys. Chem. Res., Wako, 351-01, Japan
SOURCE: Tetrahedron Letters (1991), 32(1), 101-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:164666
AB An efficient synthetic route to the glycobiosylphosphatidylinositol is developed by use of a H-phosphonate intermediate.
IT 132969-92-7P 132990-92-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 132969-92-7 CAPLUS
CN D-myo-Inositol, 6-O-[(4-methoxyphenyl)methyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate, (S)- (9CI) (CA INDEX NAME)



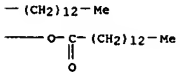
RN 132990-92-2 CAPLUS
CN D-myo-Inositol, O-2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl-(1→4)-O-2-azido-2-deoxy-3,6-bis-O-(phenylmethyl)-α-D-glucopyranosyl-(1→6)-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate], (S)- (9CI) (CA INDEX NAME)

L31 ANSWER 65 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



L31 ANSWER 66 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:58659 CAPLUS
DOCUMENT NUMBER: 114:58659
TITLE: Biosynthesis of glycosyl-phosphatidylinositol lipids in Trypanosoma brucei: involvement of mannosyl-phosphoryldolichol as the mannose donor
AUTHOR(S): Menon, Anant K.; Mayor, Satyajit; Schwarz, Ralph T.
CORPORATE SOURCE: Lab. Mol. Parasitol., Rockefeller Univ., New York, NY, 10021, USA
SOURCE: EMBO Journal (1990), 9(13), 4249-58
CODEN: EMJODG; ISSN: 0261-4189
DOCUMENT TYPE: Journal
LANGUAGE: English

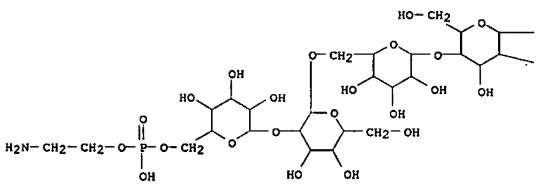
AB Trypanosome variant surface glycoproteins (VSGs) exemplify a class of eukaryotic cell-surface glycoproteins that rely on a covalently attached lipid, glycosylphosphatidylinositol, for membrane attachment. The glycolipid anchor is acquired soon after translation of the polypeptide, apparently by replacement of a short sequence of carboxyl-terminal amino acids with a precursor glycolipid. A candidate glycolipid precursor (P2) and a related glycolipid (P3) were identified in polar lipid exts. from trypanosomes. Both lipids are glycosylphosphatidylinositol species containing a Man3GlcN core glycan indistinguishable from the backbone sequence of the VSG glycolipid anchor. The cell-free synthesis of P2, P3, and a spectrum of putative biosynthetic lipid intermediates using crude prepns. of trypanosome membranes has been described. These prepns. were used to show that all three mannose residues in the glycosylphosphatidylinositol glycan are derived from dolichol-P-mannose.

IT 132237-34-4 132237-34-4D, esters with fatty acids
RL: FORM (Formation, nonpreparative)
(formation of, by Trypanosoma brucei)

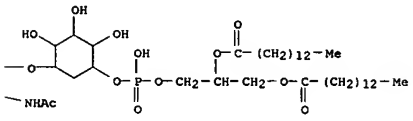
RN 132237-34-4 CAPLUS
CN myo-Inositol, O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-α-D-mannopyranosyl-(1→2)-O-α-D-mannopyranosyl-(1→6)-O-α-D-mannopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-α-D-glucopyranosyl-(1→4)-, 3-[(2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L31 ANSWER 66 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

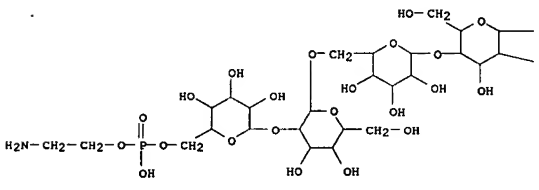


PAGE 1-B



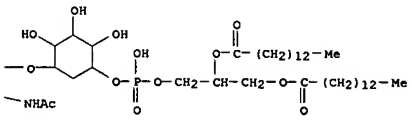
RN 132237-34-4 CAPLUS
CN myo-Inositol, O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-α-D-mannopyranosyl-(1→2)-O-α-D-mannopyranosyl-(1→6)-O-α-D-mannopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-α-D-glucopyranosyl-(1→4)-, 3-[(2R)-2,3-bis[(1-oxotetradecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

PAGE 1-A

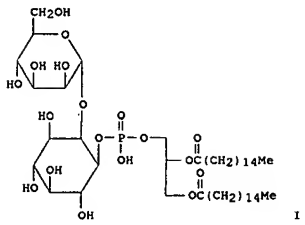


L31 ANSWER 66 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



L31 ANSWER 67 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:56485 CAPLUS
DOCUMENT NUMBER: 112:56485
TITLE: Synthesis of 1-O-(1,2-di-O-palmitoyl-sn-glycero-3-phosphoryl)-2-O-α-D-mannopyranosyl-D-myo-inositol: a fragment of mycobacterial phospholipids
AUTHOR(S): Elie, C. J. J.; Dreef, C. E.; Verduyn, R.; Van der Marel, G. A.; Van Boom, J. H.
CORPORATE SOURCE: Gorlaeus Lab., Leiden, 2300 RA, Neth.
SOURCE: Tetrahedron (1989), 45(11), 3477-86
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:56485
GI



I

AB Optically active and partially benzylated 2-O-(α-D-mannopyranosyl)-D-myo-inositol was coupled, via a trivalent phosphorus method, with 1,2-di-O-palmitoyl-sn-glycerol. Oxidation of the intermediate phosphite-triester, and subsequent removal of the P(V)- and O-benzyl protecting groups, afforded the chiral title compound I.
IT 124684-99-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to sodium salt)
RN 124684-99-7 CAPLUS
CN D-myo-Inositol,
3,4,5,6-tetrakis-O-(phenylmethyl)-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 124684-98-6
CMF C103 H137 O18 P

L31 ANSWER 67 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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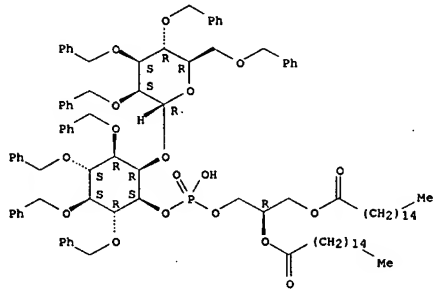
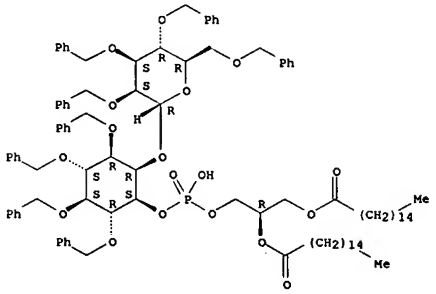


PAGE 2-A

● Na

L31 ANSWER 67 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



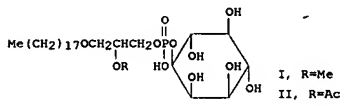
CM 2

CRN 75-64-9
CMF C4 H11 N

IT 124753-83-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 124753-83-9 CAPLUS
CN D-myo-Inositol,
3,4,5,6-tetrakis-O-(phenylmethyl)-2-O-[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

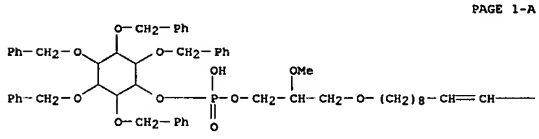
L31 ANSWER 68 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:417222 CAPLUS
DOCUMENT NUMBER: 111:17222
TITLE: Synthesis and biological evaluation of ether-linked derivatives of phosphatidylinositol
AUTHOR(S): Ishaq, Khalid S.; Capobianco, Maria; Piantadosi, Claude; Noseda, Alessandro; Daniel, Larry W.; Modest, Edward J.
CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Pharmaceutical Research (1989), 6(3), 216-24
CODEN: PHREEB; ISSN: 0724-8741
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R=Me
II, R=Ac

AB The synthesis of two novel glycero-3-phosphoinositol ether lipid analogs, racemic-1-O-octadecyl-2-O-methylglycero-3-phospho-myo-inositol (I) (an ether lipid analog of racemic-1-O-octadecyl-2-O-methylglycero-3-phosphocholine; ET-18-OMe) and racemic-1-O-octadecyl-2-O-acetylglycero-3-phospho-myo-inositol (II) (an ether lipid analog of platelet-activating factor), is described. The two target compds. and the synthetic intermediates were evaluated for inhibition of HL60, BG1, and BG3 human malignant cells in vitro and inhibition of protein kinase C. Tumor inhibitory activity was found for I and II in all systems but not for their synthetic intermediates. However, I and II as well as some synthetic intermediates exhibited protein kinase C inhibitory activity.
IT 121244-57-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antitumor activity and protein kinase C inhibition by)
RN 121244-57-3 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-methoxy-3-(9-octadecenyloxy)propyl hydrogen phosphate, (Z)- (9CI) (CA INDEX NAME)

PAGE 1-A

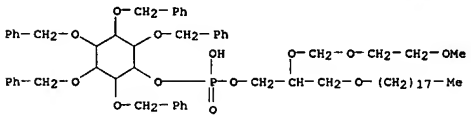


L31 ANSWER 68 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

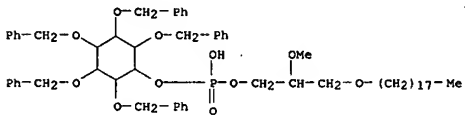
PAGE 1-B

— $(CH_2)_7$ — Me

IT 121244-54-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 121244-54-0 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-[(2-methoxyethoxy)methoxy]-3-(octadecyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)

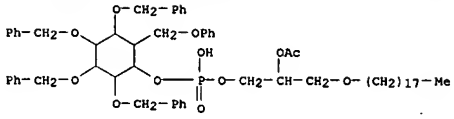


IT 121244-52-8P 121244-56-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 121244-52-8 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)



RN 121244-56-2 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-(acetyloxy)-3-(octadecyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)

L31 ANSWER 68 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

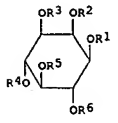


L31 ANSWER 69 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:510846 CAPLUS
DOCUMENT NUMBER: 109:110846
TITLE: Myoinositol phosphates and a process for their preparation as drugs
INVENTOR(S): Ozaki, Shoichiro; Watanabe, Yutaka; Awaya, Akira; Ishizuka, Yusaku
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 8705598 | A1 | 19870924 | WO 1987-JP149 | 19870311 |
| W: US | | | | |
| RW: CH, DE, FR, GB, IT, NL | | | | |
| JP 63198642 | A | 19880817 | JP 1987-53062 | 19870310 |
| JP 04019234 | B | 19920330 | | |
| EP 262227 | A1 | 19880406 | EP 1987-901675 | 19870311 |
| EP 262227 | B1 | 19930120 | | |
| R: CH, DE, FR, GB, IT, LI, NL | | | | |
| US 4952717 | A | 19900828 | US 1987-131049 | 19871020 |
| US 5292913 | A | 19940308 | US 1992-950760 | 19920924 |

PRIORITY APPLN. INFO.: JP 1986-51325 A 19860311
JP 1986-51326 A 19860311
JP 1986-205895 A 19860903
JP 1987-53062 A 19870310
WO 1987-JP149 W 19870311
US 1987-131049 A3 19871020
US 1990-519463 B1 19900507

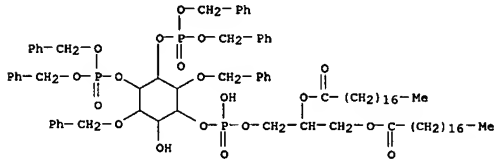
OTHER SOURCE(S): MARPAT 109:110846
GI



I

AB The title compds. [I; R1-R6 = alkyl, alkenyl, aralkyl, aryl, (un)substituted P(O)(OH)2, (un)substituted P(O)(NH2)2, SiR7R8OSiR7R8; 2 of
R1-R6 attached to adjacent OH = CR7R8, CR7OR8, SiR7R8, BR8, SnR7R8,

L31 ANSWER 69 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
P(O)XR; R = alkyl; X = O, NR; R7, R8 = alkyl, alkenylaryl, aralkyl; R7R8 =
polymethylene], useful as drugs (no data), were prepd. Treatment of 2,3,6-tri-O-benzyl-1,4,5-tri-O-allyl-sn-myoinositol with triphenylphosphine rhodium chloride in 10% aq. EtOH, refluxing the resulting 2,3,6-tri-O-benzyl-1,4,5-tri-O-(1-propenyl)-sn-myoinositol, and phosphorylation of the resulting 2,3,6-tri-O-benzyl-sn-myoinositol with dianilinophosphoric chloride in pyridine at -10°, followed by treatment with isoamyl nitrite in pyridine/Ac2O/AcOH gave 2,3,6-tri-O-benzyl-1,4,5-triphospho-sn-myoinositol which was subjected to hydrogenolysis over 5% Pd/C in aq. MeOH to give a mixt. of 1,4,5-triphosphomyoinositol and 1-phospho-4,5-pyrophosphomyoinositol.
IT 114342-79-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 114342-79-9 CAPLUS
CN D-myo-Inositol, 1,4-bis-O-(phenylmethyl)-, 3-[2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] 5,6-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)



L31 ANSWER 70 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:572785 CAPLUS
DOCUMENT NUMBER: 105:172785
TITLE: Glycerol ether phosphatides and their use
INVENTOR(S): Breuninger, Manfred; Schmidt, Dieter
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 154977 | A2 | 19850918 | EP 1985-102830 | 19850312 |
| EP 154977 | A3 | 19860219 | | |
| EP 154977 | B1 | 19890517 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| CA 1264162 | A1 | 19900102 | CA 1985-475022 | 19850225 |
| IL 74540 | A | 19890228 | IL 1985-74540 | 19850307 |
| ZA 8501774 | A | 19861029 | ZA 1985-1774 | 19850308 |
| US 4694084 | A | 19870915 | US 1985-709871 | 19850308 |
| AU 8539710 | A | 19850919 | AU 1985-39710 | 19850311 |
| AU 574440 | B2 | 19880707 | | |
| FI 8500972 | A | 19850916 | FI 1985-972 | 19850312 |
| FI 78299 | B | 19890331 | | |
| FI 78299 | C | 19890710 | | |
| AT 43131 | T | 19890615 | AT 1985-102830 | 19850312 |
| HU 36824 | A2 | 19851028 | HU 1985-923 | 19850313 |
| HU 195828 | B | 19880728 | | |
| JP 60215693 | A | 19851029 | JP 1985-48452 | 19850313 |
| DK 8501179 | A | 19850916 | DK 1985-1179 | 19850314 |
| NO 8501006 | A | 19850916 | NO 1985-1006 | 19850314 |
| ES 541242 | A1 | 19860416 | ES 1985-541242 | 19850314 |
| CN 85103123 | A | 19861022 | CN 1985-103123 | 19850423 |
| CN 1009931 | B | 19901010 | | |
| ES 550920 | A1 | 19870216 | ES 1986-550920 | 19860116 |

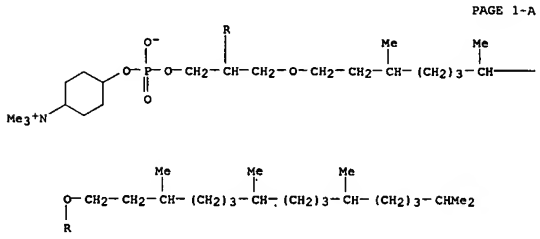
PRIORITY APPLN. INFO.: CH 1984-1287 A 19840315
CH 1985-491 A 19850204
EP 1985-102830 A 19850312

AB The title compds., useful for preparation of colloidal solns., e.g., liposome and mixed micelle solns. for drug solubilization, were prepared Thus, 2.09 mmol (RS)-2,3-bis[[(3RS,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propano 1 was added to a mixture of 8.4 mmol Et3N, CHCl3, and POCl3 at -78°, the resulting mixture cooled for 1 h and then warmed to 0°, 3.2 mmol choline tosylate in pyridine added over 30 min, and the resulting mixture stirred at room temperature for a few hours to give O-[[(RS)-2,3-bis[[(3RS,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propyl]hydroxyphosphinyl]oxy]butyl]trimethylammonium hydroxide (inner salt), 2.4 g sucrose, and 7.5 mL H2O was stirred for 1 h, the milky dispersion was sonicated for 20 min, and the resulting weakly opalescent liposome soln. was centrifuged, filtered, placed in ampuls, and heated at 120° for 20 min to give a sterilized multilamellar liposome soln.

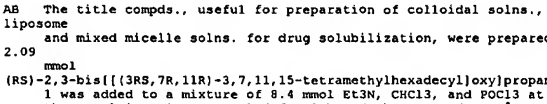
IT 103023-21-8P 103023-22-9P 103023-23-0P
103023-24-1P 103023-25-2P 103023-26-3P
103023-27-4P 103023-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for liposome)

RN 103023-21-8 CAPLUS
CN Cyclohexanaminium, 4-[[[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

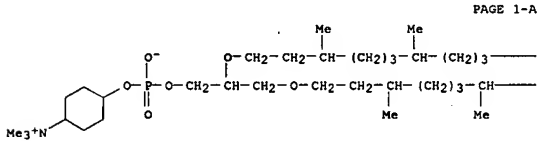


PAGE 1-B

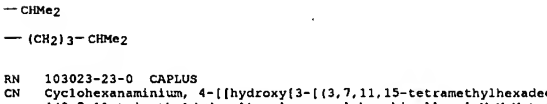


RN 103023-22-9 CAPLUS
CN Cyclohexanaminium, 4-[[[2,3-bis[(3,7,11-trimethyldodecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

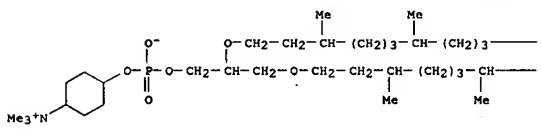


PAGE 1-B

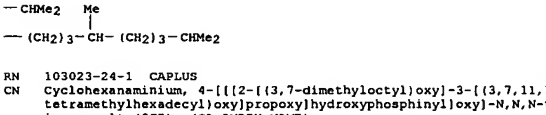


RN 103023-23-0 CAPLUS
CN Cyclohexanaminium, 4-[[hydroxy[3-[(3,7,11,15-tetramethylhexadecyl)oxy]-2-[(3,7,11-trimethyldodecyl)oxy]propoxy]phosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

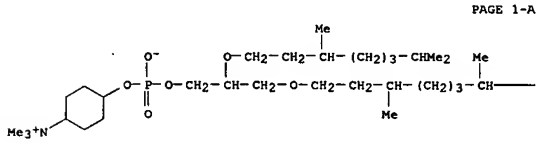


PAGE 1-B

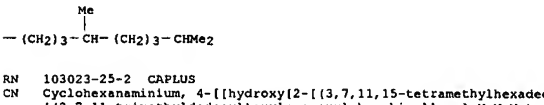


RN 103023-24-1 CAPLUS
CN Cyclohexanaminium, 4-[[[2-[(3,7-dimethyloctyl)oxy]-3-[(3,7,11,15-tetramethylhexadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

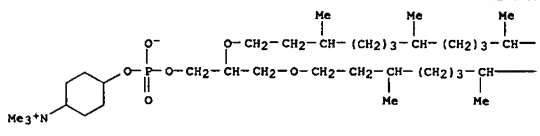


PAGE 1-B

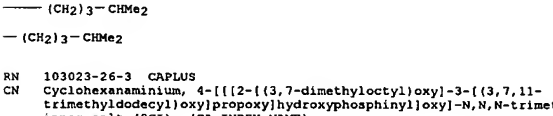


RN 103023-25-2 CAPLUS
CN Cyclohexanaminium, 4-[[hydroxy[2-[(3,7,11,15-tetramethylhexadecyl)oxy]-3-[(3,7,11-trimethyldodecyl)oxy]propoxy]phosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



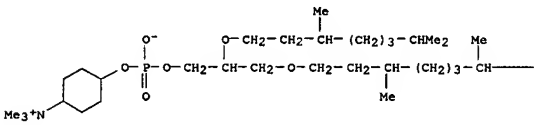
PAGE 1-B



RN 103023-26-3 CAPLUS
CN Cyclohexanaminium, 4-[[[2-[(3,7-dimethyloctyl)oxy]-3-[(3,7,11-trimethyldodecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

L31 ANSWER 70 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

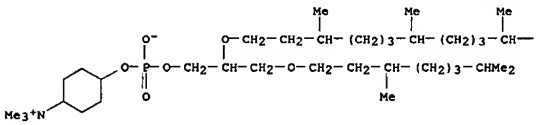


PAGE 1-B

— $(CH_2)_3$ — $CHMe_2$

RN 103023-27-4 CAPLUS
CN Cyclohexanaminium, 4-[[[3-[(3,7-dimethyloctyl)oxy]-2-[(3,7,11,15-tetramethylhexadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— $(CH_2)_3$ — $CHMe_2$

RN 103023-28-5 CAPLUS
CN Cyclohexanaminium, 4-[[[3-[(3,7-dimethyloctyl)oxy]-2-[(3,7,11-trimethyldodecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

L31 ANSWER 71 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN

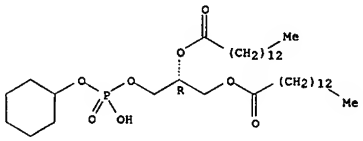
ACCESSION NUMBER: 1985:77260 CAPLUS
DOCUMENT NUMBER: 102:77260
TITLE: Primary or secondary alcohol derivatives of phospholipids produced by the enzymic technique
INVENTOR(S): Kokusho, Yoshitaka; Kato, Shigeaki; Machida, Haruo
PATENT ASSIGNEE(S): Meito Sangyo Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 80 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 122151 | A2 | 19841017 | EP 1984-302444 | 19840410 |
| EP 122151 | A3 | 19860326 | | |
| EP 122151 | B1 | 19890215 | | |
| R: CH, DE, FR, GB, IT, LI, NL | | | | |
| JP 59187786 | A | 19841024 | JP 1983-63305 | 19830411 |
| JP 02008716 | B | 19900226 | | |
| JP 60041494 | A | 19850305 | JP 1983-63304 | 19830411 |
| JP 02007633 | B | 19900220 | | |
| US 4783402 | A | 19881108 | US 1984-598697 | 19840410 |
| PRIORITY APPLN. INFO.: | | | JP 1983-63304 A | 19830411 |
| | | | JP 1983-63305 A | 19830411 |

OTHER SOURCE(S): MARPAT 102:77260
AB Primary and secondary alc. derivs. of phospholipids are produced by reacting the alc. with a lecithin, catalyzed by phospholipase [9013-93-8]
DM from Nocardiopsis or Actinomadura. Thus, 400 mg β-γ-dihexadecyl-L-α-lecithin [36314-47-3] was emulsified in 1 mL ether and 10 mL H2O. Then, 2 mL emulsion was mixed with 2 mL pH 5.7 0.4M acetate buffer, 1 mL 0.1M CaCl2, 2 mL 10% solution of thiamin [59-43-8] HCl
in ether, and 2 mL aqueous solution of phospholipase DM (2.5 units/mL) and let
stand at 37° for 3 h. The yield of the thiamin derivative of 1,2-dihexadecyl-sn-glycerol 3-phosphoric acid [94475-74-8] was 30 mg.
IT 94456-54-9P 94456-55-0P 94456-72-1P
94456-73-2P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, from lecithin and alc., enzymic)
RN 94456-54-9 CAPLUS
CN Tetradecanoic acid, 1-[[[(cyclohexyloxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester, (R)- (9CI) (CA INDEX NAME)

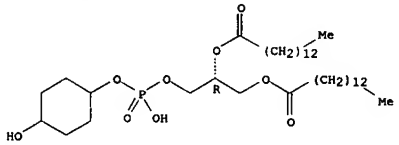
Absolute stereochemistry.

L31 ANSWER 71 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



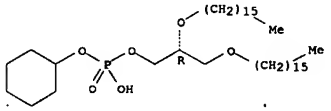
RN 94456-55-0 CAPLUS
CN Tetradecanoic acid, 1-[[[hydroxy[(4-hydroxycyclohexyl)oxy]phosphinyl]oxy]methyl]-1,2-ethanediyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 94456-72-1 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] monocyclohexyl ester, (R)- (9CI) (CA INDEX NAME)

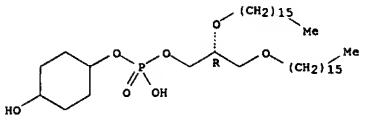
Absolute stereochemistry.



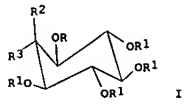
RN 94456-73-2 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono(4-hydroxycyclohexyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 71 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

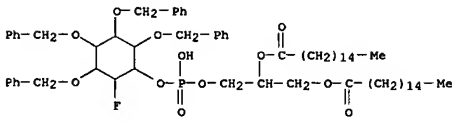


L31 ANSWER 72 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:215923 CAPLUS
DOCUMENT NUMBER: 98:215923
TITLE: Synthesis of fluorodeoxyscylloinositol and phosphatidylfluorodeoxyscylloinositol
AUTHOR(S): Yang, Shu Shu; Beattie, Thomas R.; Shen, T. Y.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Div. Merck and Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Tetrahedron Letters (1982), 23(52), 5517-20
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

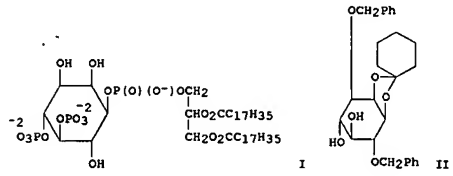


AB Fluorination of myoinositol derivative I (R = Bz, R1 = PhCH2, R2 = OH, R3 = H) by DAST in PhMe at 70-80° followed by aqueous work-up gave 86% I (R, R1 as before, R2 = H, R3 = F), which on mild hydrolysis gave 95% I (R = R2 = H, R1 = PhCH2, R3 = F) (II). Debenzylation of II in aqueous EtOH in the presence of Pd black gave I (R-R2 = H, R3 = F), quant. Condensation reaction of II with Me(CH2)14CO2CH[CH2O2C(CH2)14Me]CH2OP(O)(ONa)2 followed by hydrogenolysis gave I [R = Me(CH2)14CO2CH2CH[O2C(CH2)14Me]CH2OP(O)(OH), R1 = R2 = H, R3 = F] in high yield.
IT 85747-86-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 85747-86-0 CAPLUS
CN scyllo-Inositol, 1-deoxy-1-fluoro-2,3,4,5-tetrakis-O-(phenylmethyl)-, 2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate, (S)- (9CI) (CA INDEX NAME)

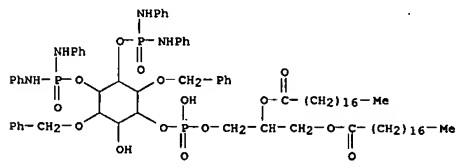
L31 ANSWER 72 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



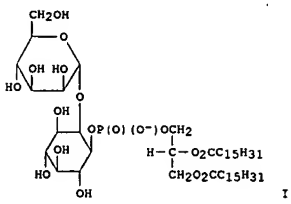
L31 ANSWER 73 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:593546 CAPLUS
DOCUMENT NUMBER: 91:193546
TITLE: Synthesis of a triphosphoinositide
AUTHOR(S): Krylova, V. N.; Gornaeva, N. P.; Shvets, V. I.; Evstigneeva, R. P.
CORPORATE SOURCE: Mosk. Inst. Tonk. Khim. Tekhnol., Moscow, USSR
SOURCE: Doklady Akademii Nauk SSSR (1979), 246(2), 339-40 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



AB The title compound I was prepared in 5 steps from II by treatment with (PhNH)2P(O)Cl, deacetalization, condensation with 1,2-di-O-stearoyl-3-O-phosphoglycerin, and debenzylation and treatment with isoamyl nitrite.
IT 71788-35-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)
RN 71788-35-7 CAPLUS
CN myo-Inositol, 3,6-bis-O-(phenylmethyl)-, 1-[2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] 4,5-bis(N,N'-diphenylphosphorodiamidate) (9CI) (CA INDEX NAME)



L31 ANSWER 74 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:601949 CAPLUS
DOCUMENT NUMBER: 87:201949
TITLE: Studies of derivatives of asymmetrically substituted myo-inositol. XIX. Synthesis of 1-O-(1,2-di-O-palmitoyl-sn-glycero-3-O-phosphoryl)-2-O-α-D-mannopyranosyl-sn-myo-inositol
AUTHOR(S): Stepanov, A. E.; Shvets, V. I.; Evstigneeva, R. P.
CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SOURCE: Zhurnal Obshchei Khimii (1977), 47(7), 1653-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

AB The title compound I was obtained in 65.5% yield as its ammonium salt by phosphorylation of (tetraacetylmannopyranosyl)tetrabenzylmyoinositol with the corresponding phosphatidic acid followed by deacetylation-debenzylation.
IT 64697-09-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, deacetylation, and debenzylation of)
RN 64697-09-2 CAPLUS
CN D-myo-Inositol, 3,4,5,6-tetrakis-O-(phenylmethyl)-2-O-(2,3,4,6-tetra-O-acetyl-α-D-mannopyranosyl)-, (2R)-2,3-bis[(1-oxohexadecyl)oxy]propyl hydrogen phosphate (9CI) (CA INDEX NAME)

L31 ANSWER 74 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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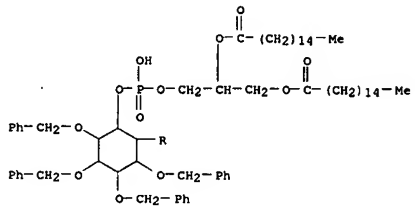
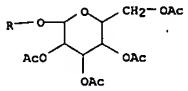
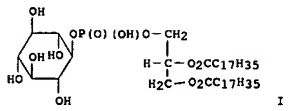


PAGE 2-A

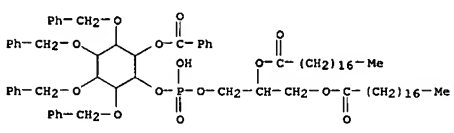


L31 ANSWER 75 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:190385 CAPLUS
DOCUMENT NUMBER: 86:190385
TITLE: Synthesis of phosphatidyl-scyllo-inositol
AUTHOR(S): Shevchenko, V. P.; Lazurkina, T. Yu.; Molotkovskii, Yu. G.; Bergel'son, L. D.
CORPORATE SOURCE: M. M. Shemyakin Inst. Bioorg. Chem., Moscow, USSR
SOURCE: Bioorganicheskaya Khimiya (1977), 3(2), 252-5
CODEN: BIKHD7; ISSN: 0132-3423
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

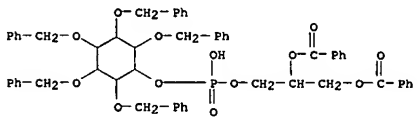


I

AB The title compound I was obtained in 35% yield in 4 steps from myo-inositol
II by oxidation with CrO3, reduction with NaBH4 to give the scyllo isomer,
treatment with 1,2-distearoylglycerophosphate, and removal of the protecting groups.
IT 62700-85-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and removal of protecting groups from)
RN 62700-85-0 CAPLUS
CN scyllo-Inositol, 1,2,3,4-tetrakis-O-(phenylmethyl)-, 5-benzoate 6-[2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



L31 ANSWER 76 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:449948 CAPLUS
DOCUMENT NUMBER: 81:49948
TITLE: Synthetic routes for natural phosphoinositols
AUTHOR(S): Shevts, V. I.; Klyashchitskii, B. A.; Zhelvakova, E. G.; Stepanov, A. E.
CORPORATE SOURCE: USSR
SOURCE: Khim. Khim. Tekhnol., Tr. Yubileinoi Konf., Posvyashch. 70-Letiyu Inst. (Mosk. Inst. Tonkoi Khim. Tekhnol.) (1972), Meeting Date 1970, 138-40.
Editor(s): Bashkirov, A. N. Mosk. Inst. Tonkoi Khim. Tekhnol.: Moscow, USSR.
CODEN: 28IMAS
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Phosphoinositol (I) was prepared from 2,3,4,5,6-penta-O-benzyl-sn-myo-inositol followed by debenzylation. Addnl. obtained was mannopyranosylinositol (II).
IT 53115-98-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53115-98-3 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2,3-bis(benzoyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)



L31 ANSWER 77 OF 77 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:3819 CAPLUS
DOCUMENT NUMBER: 74:3819
TITLE: Synthesis of phosphatidylinositol
AUTHOR(S): Gent, Patricia A.; Gigg, Roy; Warren, Christopher D.
CORPORATE SOURCE: Nat. Inst. Med. Res., London, UK
SOURCE: Tetrahedron Letters (1970), (30), 2575-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:3819
GI For diagram(s), see printed CA Issue.
AB I (R = Ag, R1 = CH2Ph) was condensed with optically active Me(CH2)14CO2CH2CH[O2C(CH2)14Me]CH2I (Ia) to give II (R = R1 = CH2Ph) which upon treatment with NaI gave II (R = Na, R1 = CH2Ph). II (R = H, R1 = CH2Ph) gave upon hydrogenation a diastereoisomeric mixture of phosphatidylinositols [II; R = R1 = H]. In the 2nd method II (R = H, R1 = CH2Ph) was prepared directly from I (R = R1 = H) by condensation with 1,2-di-O-palmitoyl-L-glycerol in the presence of triisopropyl-benzenesulfonyl chloride. Condensation of I (R = Ag, R1 = Ph) with Ia gave II (R = Ph, R1 = CH2Ph) which upon hydrogenation with Pd/C gave II (R = Ph, R1= H). The latter upon hydrogenation with Pd gave a mixture of products including diglycerides. The hydrogenolysis of II (R = H, R1 = CH2Ph) gave quant. II (R = R1 = H).
IT 30785-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30785-82-1 CAPLUS
CN Inositol, 1,2,4,5,6-penta-O-benzyl-, dihydrogen phosphate, monoester with L-1,2-dipalmitin, myo- (8CI) (CA INDEX NAME)